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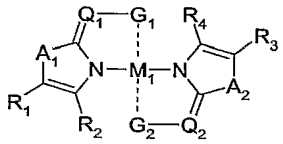
(54) Title: OPTICAL RECORDING MATERIALS HAVING HIGH STORAGE DENSITY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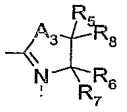
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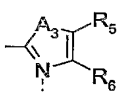
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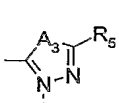
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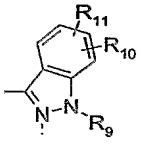
(XII)

(57) Abstract: The invention relates to an optical recording medium comprising a substrate, a reflecting layer and a recording layer based on compounds of formula (I) wherein G_1 and G_2 are each independently of the other, A_1 and A_2 are each independently of the other $N(R_{12})$, O, S or Se and A_3 is $C(C_1\text{-}C_5\text{alkyl})_2$, $C(C_4\text{-}C_5$ alkylene), $N(R_{12})$, O, S, Se, $N{=}C(R_{13})$ or unsubstituted or R_{14}-substituted CH=CH; M_1 is a transition metal of groups (IX) to (XII), preferably Co, Cu, Ni, Pd or Zn, especially Co, Cu or Ni; Q_1 and Q_2 are each independently of the other $C(R_{15})$, N or P,... For the detailed definitions of the further substituents, see the description. Recording and playback are effected especially at a wavelength of from 350 to 500 nm, for example using a blue laser. The recording and playback quality is excellent and allows a high storage density. Also claimed are new compounds of formula (I), with the exception of the compounds disclosed in J. Org. Chem. 67/16, 5753-5772 [2002].

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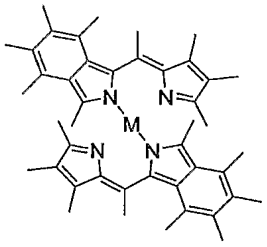
Optical recording materials having high storage density

The invention relates to new optical recording materials that have excellent recording and playback quality especially at a wavelength of 350-500 nm. Recording and playback can be effected very advantageously with high sensitivity at the same wavelength, and the storage density that is achievable is significantly higher than in the case of known materials. In addition, the materials according to the invention have very good storage properties before and after recording, even under especially harsh conditions, such as exposure to sunlight or fluorescent lighting, heat and/or high humidity. In addition, their manufacture is simple and readily reproducible using customary coating processes, such as spin-coating.

WO 02/082438 discloses the use of ionic salts, including those with metal complex anions, for optical recording materials. Those colorants are always substituted by alkyl, alkenyl, aryl or heteroaryl at the nitrogen atom. Their optical properties do not, however, fully satisfy increased demands. In particular, the refractive index as well as the absorption and the steepness of the absorption band on its long wavelength flank in the solid still leave something to be desired.

JP-A-11/34500, JP-A-11/92479 and EP-A-0 903 733 disclose metal and boron complexes of colorants of formulae  and



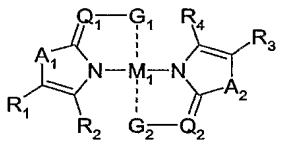
, which can be used at from 520 to 690 nm for optical recording materials such as CD-R or DVD-R. Here too, however, the optical

properties, especially the spectral properties in or near the UV range that are necessary for the highest possible storage densities, and the information density per unit surface area are not able to satisfy the highest demands as desired. The information density per unit surface area is far lower than is desirable.

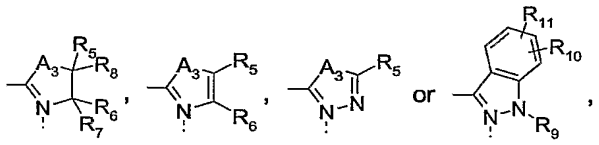
Conventional optical recording materials therefore satisfy high demands only to some extent, or do not satisfy all demands to an entirely satisfactory degree at the same time.

On the other hand, J. Org. Chem. 67/16, 5753-5772 [2002] describes the synthesis of a number of bis(*o*-azaheteroaryl)methanes and their coordination properties with respect to divalent transition metals, heteroaryl being 1,3-azol-2-yl, 1,3-benzazol-2-yl and azinyl and the transition metals being Zn, Cu, Co, Ni, Hg and Pd. *Inter alia* 2:1 salt complexes of bis(benzothiazol-2-yl)methane and bis(benzoxazol-2-yl)methane with copper(II) chloride and nickel(II) sulfate, and cobalt(II) chloride and palladium(II) nitrate are disclosed, whereas bis(thiazol-2-yl)methane yields, with deprotonation, neutral 2:1 chelates with Zn(II), Cu(II), Ni(II) and Co(II). All substances are strongly coloured.

The aim of the invention is an optical recording medium having high information density, sensitivity and data reliability. Such a recording medium should be robust, durable and easy to use. Furthermore, it should be inexpensive to manufacture as a mass-produced product and should require equipment that is as small and inexpensive as possible.

The invention therefore relates to an optical recording medium comprising a substrate, a recording layer and optionally one or more reflecting layers, wherein the recording layer comprises a compound of formula  (I) or a tautomer thereof, wherein

G_1 and G_2 are each independently of the other

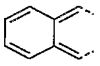


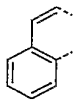
A_1 and A_2 are each independently of the other $N(R_{12})$, O, S or Se and A_3 is $C(C_1\text{-}C_5alkyl)_2$, $C(C_4\text{-}C_5alkylene)$, $N(R_{12})$, O, S, Se, $N{=}C(R_{13})$ or unsubstituted or R_{14}-substituted CH=CH;

M_1 is a transition metal of groups IX to XII, preferably Co, Cu, Ni, Pd or Zn, especially Co, Cu or Ni;

Q_1 and Q_2 are each independently of the other $C(R_{15})$, N or P;

R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8 and R_{14} are each independently of the others hydrogen, R_{18}, or $C_6\text{-}C_{12}aryl$, $C_4\text{-}C_{12}heteroaryl$, $C_7\text{-}C_{12}aralkyl$ or $C_5\text{-}C_{12}heteroaralkyl$ each unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18}; or

R_1 and R_2, R_3 and R_4, R_5 and R_6, R_5 and R_{13} and/or R_5 and R_{14}, together in pairs, are $C_3\text{-}C_6alkylene$ or $C_3\text{-}C_6alkenylene$, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17} and may be uninterrupted or interrupted by O, S or $N(R_{12})$, or 1,4-buta-1,3-dienylene, 

or  , each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18} and in which 1 or 2 carbon atoms may have been replaced by nitrogen;

R_9, R_{12} and R_{13} are each independently of the others C_1-C_{24}alkyl, C_3-C_{24}cycloalkyl, C_2-C_{24}alkenyl, C_3-C_{24}cycloalkenyl, C_1-C_4alkyl-[O-C_1-C_4alkylene]$_m$ or C_1-C_4alkyl-[NH-C_1-C_4alkylene]$_m$, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17}; or C_6-C_{12}aryl, C_4-C_{12}heteroaryl, C_7-C_{12}aralkyl or C_5-C_{12}heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18};

R_{10}, R_{11} and R_{18} are each independently of the others halogen, nitro, cyano, thiocyanato, hydroxy, O-R_{19}, O-CO-R_{19}, S-R_{19}, CHO, COR_{20}, $CHOR_{19}OR_{23}$, $CR_{20}OR_{19}OR_{23}$, R_{16}, N=N-R_{16}, N=$CR_{19}R_{20}$, N=$CR_{21}R_{22}$, C(R_{15})=NR_{19}, C(R_{15})=NR_{21}, C(R_{15})=$CR_{21}R_{22}$, NH_2, NH-R_{19}, $NR_{19}R_{20}$, NH_3^+, $NH_2R_{19}^+$, $NHR_{19}R_{20}^+$, $NR_{19}R_{20}R_{23}^+$, $CONH_2$, $CONHR_{19}$, $CONR_{19}R_{20}$, SO_2R_{19}, SO_2NH_2, SO_2NHR_{19}, $SO_2NR_{19}R_{20}$, COOH, $COOR_{19}$, $OCOOR_{19}$, $NHCOR_{19}$, $NR_{19}COR_{23}$, $NHCOOR_{19}$, $NR_{19}COOR_{23}$, ureido, NR_{19}-CO-NHR_{23}, $B(OH)_2$, $B(OH)(OR_{19})$, $B(OR_{19})OR_{23}$, phosphato, $PR_{19}R_{23}$, $POR_{19}OR_{23}$, P(=O)$OR_{19}OR_{23}$, $OPR_{19}R_{23}$, $OPR_{19}OR_{23}$, OP(=O)$R_{19}OR_{23}$, OP(=O)$OR_{19}OR_{23}$, OPO_3R_{19}, sulfato, sulfo, or C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_1-C_{12}alkylthio, C_3-C_{12}cycloalkylthio, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy each unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17};

R_{15} is hydrogen, cyano, hydroxy, C_1-C_{12}alkoxy, C_3-C_{12}cycloalkoxy, C_1-C_{12}alkylthio, C_3-C_{12}cycloalkylthio, amino, NHR_{24}, $NR_{25}R_{26}$, R_{27}, halogen, nitro, formyl, N=N-R_{27}, C(R_{14})=$CR_{21}R_{22}$, C(R_{14})=NR_{19}, COO-R_{25}, carboxy, carbamoyl, CONH-R_{25}, $CONR_{25}R_{26}$, N=$CR_{19}R_{20}$, or C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_2-C_{12}alkenyl or C_3-C_{12}cycloalkenyl each unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy radicals;

R_{16} is C_6-C_{12}aryl, C_4-C_{12}heteroaryl, C_7-C_{12}aralkyl or C_5-C_{12}heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{28};

R_{17} is halogen, hydroxy, O-R_{25}, O-CO-R_{25}, S-R_{25}, NH_2, NH-R_{25}, $NR_{25}R_{26}$, NH_3^+, $NH_2R_{25}^+$, $NHR_{25}R_{26}^+$, $NR_{24}R_{25}R_{26}^+$, NR_{25}-CO-R_{24}, $NR_{25}COOR_{24}$, cyano, formyl, COO-R_{25}, carboxy, carbamoyl, CONH-R_{25}, $CONR_{25}R_{26}$, ureido, NH-CO-NHR_{24}, NR_{25}-CO-NHR_{24}, phosphato, $PR_{25}R_{24}$, $POR_{25}OR_{24}$, $P(=O)OR_{25}OR_{24}$, $OPR_{25}R_{24}$, $OPR_{25}OR_{24}$, $OP(=O)R_{25}OR_{24}$, OPO_3R_{25}, $OP(=O)OR_{25}OR_{24}$, SO_2R_{25}, sulfato, sulfo, R_{27}, N=N-R_{27}, or C_1-C_{12}alkoxy or C_1-C_{12}cycloalkoxy each unsubstituted or mono- or poly-substituted by halogen;

R_{19}, R_{20} and R_{23} are each independently of the others R_{16}, or C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_2-C_{12}alkenyl or C_3-C_{12}cycloalkenyl each unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy radicals; or

R_{14} and R_{19} together, R_{15} and R_{19} together and/or R_{19} and R_{23} together are C_2-C_{12}alkylene, C_3-C_{12}cycloalkylene, C_2-C_{12}alkenylene or C_3-C_{12}cycloalkenylene, each of which is unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy radicals; or

R_{19} and R_{20} together with the common nitrogen are pyrrolidine, piperidine, piperazine or morpholine, each of which is unsubstituted or mono- to tetra-substituted by C_1-C_4alkyl; or carbazole, phenoxazine or phenothiazine, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{28};

R_{21} and R_{22} are each independently of the other $NR_{25}R_{26}$, CN, $CONH_2$, $CONHR_{19}$, $CONR_{19}R_{20}$ or $COOR_{20}$;

R_{24}, R_{25} and R_{26} are each independently of the others C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_2-C_{12}alkenyl, C_3-C_{12}cycloalkenyl, C_6-C_{12}aryl, C_4-C_{12}heteroaryl, C_7-C_{12}aralkyl or C_5-C_{12}heteroaralkyl; or

R_{25} and R_{26} together with the common nitrogen are pyrrolidine, piperidine, piperazine or morpholine, each of which is unsubstituted or mono- to tetra-substituted by C_1-C_4alkyl;

R_{27} is C_6-C_{12}aryl, C_4-C_{12}heteroaryl, C_7-C_{12}aralkyl or C_5-C_{12}heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18};

R_{28} is nitro, SO_2NHR_{25}, $SO_2NR_{25}R_{26}$, or C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_1-C_{12}alkylthio, C_3-C_{12}cycloalkylthio, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy each unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17}; and

m is a number from 1 to 10.

When R_5 forms a bridge with R_6, R_5 may not at the same time form a bridge with R_{13} or R_{14}.

It will be understood that acidic groups, such as carboxy, sulfo, sulfato and phosphato, may also be in the form of a salt, for example an alkali metal, alkaline earth metal, ammonium or phosphonium salt, such as Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}, Cu^{2+}, Ni^{2+}, Fe^{2+}, Co^{2+}, Zn^{2+}, Sn^{2+}, La^{3+}, ammonium, methylammonium, ethylammonium, isopropylammonium, ™Primene 81-R, ™Rosin Amine D, pentadecylammonium, ™Primene JM-T, dicyclohexylammonium, tetramethylammonium, tetraethylammonium, tetrabutylammonium, benzyltrimethylammonium, benzyltriethylammonium, methyltrioctylammonium, tridodecylmethylammonium, tetrabutylphosphonium, tetraphenylphosphonium, butyltriphenylphosphonium or ethyltriphenylphosphonium, or any of the cations B-1 to B-169 mentioned in US-6 225 024, to which individually reference is expressly made here.

Halogen is chlorine, bromine, fluorine or iodine, preferably fluorine or chlorine, especially fluorine on alkyl (for example trifluoromethyl, α,α,α-trifluoroethyl or perfluorinated alkyl groups, such as heptafluoropropyl) and chlorine on aryl,

heteroaryl or on the aryl moiety of aralkyl or on the heteroaryl moiety of hetero-aralkyl.

Alkyl, cycloalkyl, alkenyl or cycloalkenyl can be straight-chain or branched, or monocyclic or polycyclic. Alkyl is, for example, methyl, straight-chain C_2-C_{24}alkyl or preferably branched C_3-C_{24}alkyl. Alkenyl is, for example, straight-chain C_2-C_{20}alkenyl or preferably branched C_3-C_{24}alkenyl. The invention therefore relates especially also to compounds of formula (I) containing branched C_3-C_{24}alkyl or branched C_3-C_{24}alkenyl, and also to optical recording materials comprising such compounds. C_1-C_{24}Alkyl is therefore, for example, methyl, ethyl, n-propyl, isopropyl, n-butyl, sec-butyl, isobutyl, tert-butyl, n-pentyl, 2-pentyl, 3-pentyl, 2,2-dimethylpropyl, n-hexyl, n-octyl, 1,1,3,3-tetramethylbutyl, 2-ethylhexyl, nonyl, decyl, dodecyl, tetradecyl, hexadecyl, octadecyl, eicosyl, heneicosyl, docosyl or tetracosyl. C_3-C_{24}Cycloalkyl is, for example, cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, trimethylcyclohexyl, menthyl, thujyl, bornyl, 1-adamantyl or 2-adamantyl.

C_2-C_{20}Alkenyl and C_3-C_{20}cycloalkenyl are C_2-C_{20}alkyl and C_3-C_{20}cycloalkyl that is mono- or poly-unsaturated, wherein two or more double bonds may be isolated or conjugated, for example vinyl, allyl, 2-propen-2-yl, 2-buten-1-yl, 3-buten-1-yl, 1,3-butadien-2-yl, 2-cyclobuten-1-yl, 2-penten-1-yl, 3-penten-2-yl, 2-methyl-1-buten-3-yl, 2-methyl-3-buten-2-yl, 3-methyl-2-buten-1-yl, 1,4-pentadien-3-yl, 2-cyclopenten-1-yl, 2-cyclohexen-1-yl, 3-cyclohexen-1-yl, 2,4-cyclohexadien-1-yl, 1-*p*-menthen-8-yl, 4(10)-thujen-10-yl, 2-norbornen-1-yl, 2,5-norbornadien-1-yl, 7,7-dimethyl-2,4-norcaradien-3-yl or the various isomers of hexenyl, octenyl, nonenyl, decenyl, dodecenyl, tetradecenyl, hexadecenyl, octadecenyl, eicosenyl, heneicosenyl, docosenyl, tetracosenyl, hexadienyl, octadienyl, nonadienyl, decadienyl, dodeca-dienyl, tetradecadienyl, hexadecadienyl, octadecadienyl or eicosadienyl.

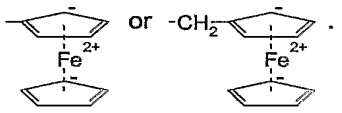
C_7-C_{12}Aralkyl is, for example, benzyl, 2-benzyl-2-propyl, β-phenyl-ethyl, 9-fluorenyl, α,α-dimethylbenzyl, ω-phenyl-butyl or ω-phenyl-hexyl. When C_7-C_{12}aralkyl is substituted, both the alkyl moiety and the aryl moiety of the aralkyl group can be

substituted, the latter alternative being preferred.

C_6-C_{12}Aryl is, for example, phenyl, naphthyl, biphenylyl or 2-fluorenyl.

C_4-C_{12}Heteroaryl is an unsaturated or aromatic radical having 4n+2 conjugated π-electrons, for example 2-thienyl, 2-furyl, 2-pyridyl, 2-thiazolyl, 2-oxazolyl, 2-imidazolyl, isothiazolyl, triazolyl or any other ring system consisting of thiophene, furan, pyridine, thiazole, oxazole, imidazole, isothiazole, triazole, pyridine and benzene rings and unsubstituted or substituted by from 1 to 6 ethyl, methyl, ethylene and/or methylene substituents, for example benzotriazolyl, and in the case of N-heterocycles where applicable also those in the form of their N-oxides.

C_5-C_{12}Heteroaralkyl is, for example, C_1-C_8alkyl substituted by C_4-C_{11}heteroaryl.

Furthermore, aryl and aralkyl can also be aromatic groups bonded to a metal, for example in the form of metallocenes of transition metals known *per se*, more especially  or .

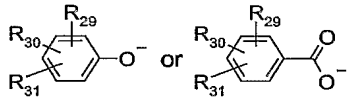
The transition metal M_1 is preferably in the form of a doubly positively charged cation, for example Co^{2+}, Cu^{2+}, Ni^{2+}, Pd^{2+} or Zn^{2+}, especially Co^{2+}, Cu^{2+} or Ni^{2+}.

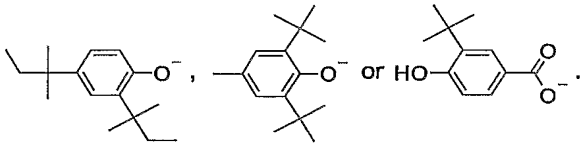
The compound of formula (I) may also be a cation which has been neutralised with an inorganic, organic or organometallic anion, for example when one or more ammonium groups are present or when the transition metal has one or more excess positive charges, such as in Co^{3+}. The inorganic, organic or organometallic anion may be, for example, the anion of a mineral acid, of the conjugated base of an organic acid (for example an alcoholate, phenolate, carboxylate, sulfonate or phosphonate) or an organometallic complex anion, for example fluoride, chloride, bromide, iodide, perchlorate, periodate, nitrate, hydrogen carbonate, ½ carbonate, ½ sulfate, C_1-C_4alkyl sulfate, hydrogen sulfate, ⅓ phosphate, ½ hydrogen phos-

phate, dihydrogen phosphate, ½ C_1-C_4alkanephosphonate, C_1-C_4alkane-C_1-C_{12}alkylphosphonate, di-C_1-C_4alkylphosphinate, tetrafluoroborate, hexafluorophosphate, hexafluoroantimonate, acetate, trifluoroacetate, heptafluorobutyrate, ½ oxalate, methanesulfonate, trifluoromethanesulfonate, benzenesulfonate, tosylate, p-chlorobenzenesulfonate, p-nitrobenzenesulfonate, phenolate, benzoate or a negatively charged metal complex.

The person skilled in the art will readily recognise that it is also possible to use other anions with which he is familiar. It will be self-evident to him that $\frac{1}{x}$ of an inorganic, organic or organometallic anion having x negative charges, for example ½· SO_4^{2-}, is a multiply charged anion which neutralises several singly charged cations or a cation having x charges, as the case may be.

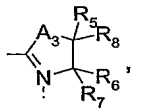
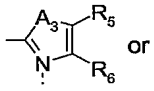
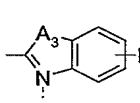
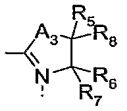
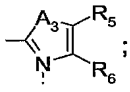
Phenolates or carboxylates are, for example, of formula

 (wherein R_{29}, R_{30} and R_{31} are each independently of the others hydrogen, R_{18}, or C_6-C_{12}aryl, C_4-C_{12}heteroaryl, C_7-C_{12}aralkyl or C_5-C_{12}heteroaralkyl each unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18}, for example anions of C_1-C_{12}alkylated, especially tert-C_4-C_8alkylated, phenols and benzoic acids, such as



Preference is given to compounds of formula (I) wherein

A_1, A_2 and A_3 are each independently of the others O, S or N(R_{12}) and/or Q_1 and Q_2 are C(R_{15}) or N;

G_1 and G_2 are each independently of the other  ,  or  , especially  or  ;

R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8 and R_{14} are each independently of the others hydrogen, R_{18}, or C_6-C_{12}aryl or C_7-C_{12}aralkyl each unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18};

R_9, R_{12} and R_{13} are each independently of the others unsubstituted or R_{17}-substituted C_1-C_8alkyl;

R_{10} and R_{18} are each independently of the other halogen, nitro, cyano, O-R_{19}, formyl, $CH=C(CN)_2$, $CH=C(CN)CONH_2$, $CH=C(CN)CONHR_{19}$, $CH=C(CN)CONR_{19}R_{20}$, $CH=C(CN)COOR_{19}$, $CH=C(COOR_{19})COOR_{20}$, $CONH_2$, $CONHR_{19}$, $CONR_{19}R_{20}$, SO_2C_1-C_{12}alkyl, SO_2NH_2, SO_2NHR_{19}, $SO_2NR_{19}R_{20}$, COOH, $COOR_{19}$, $NHCOR_{19}$, $NR_{19}COR_{23}$, $NHCOOR_{19}$, $NR_{19}COOR_{23}$, ureido, $P(=O)OR_{19}OR_{23}$, sulfo, or C_1-C_{12}alkyl, C_1-C_{12}alkylthio or C_1-C_{12}alkoxy each unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17};

R_{15} is hydrogen, cyano, halogen, nitro, formyl, $N=N-R_{27}$, $C(R_{14})=CR_{21}R_{22}$, $C(R_{14})=NR_{19}$, $COO-R_{25}$, carboxy, carbamoyl, $CONH-R_{25}$, $CONR_{25}R_{26}$, or C_1-C_{12}alkyl unsubstituted or substituted by one or more halogen substituents;

R_{16} is unsubstituted or substituted C_6-C_{12}aryl or C_7-C_{12}aralkyl, especially a metallocenyl radical;

R_{17} is halogen, hydroxy, O-R_{25}, amino, NH-R_{25}, $NR_{25}R_{26}$, NR_{25}-CO-R_{24}, $NR_{25}COOR_{24}$, cyano, $COO-R_{25}$, carboxy, $CONH-R_{25}$, $CONR_{25}R_{26}$, sulfato, sulfo, or C_1-C_{12}alkoxy unsubstituted or mono- or poly-substituted by halogen;

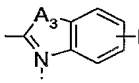
R_{19}, R_{20} and R_{23} are each independently of the others C_1-C_{12}alkyl unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy or C_1-C_{12}alkoxy radicals, or unsubstituted C_6-C_{12}aryl or C_7-C_{12}aralkyl; or

R_{19} and R_{20} together with the common nitrogen are morpholine, or piperidine N-substituted by C_1-C_4alkyl;

R_{25}, R_{26} and R_{24} are each independently of the others C_1-C_{12}alkyl, C_2-C_{12}alkenyl, C_6-C_{12}aryl or C_7-C_{12}aralkyl; or

R_{25} and R_{26} together with the common nitrogen are morpholine, or piperidine N-substituted by C_1-C_4alkyl; and/or

m is a number from 1 to 4.

Special preference is given to compounds of formula (I) wherein Q_1 and Q_2 are $C(R_{15})$; G_1 and G_2 are  ; and A_1, A_2 and A_3 are O, S or $N(R_{12})$;

R_{12} is C_1-C_{24}alkyl, C_1-C_4alkyl-[O-C_1-C_4alkylene]$_m$ or C_1-C_4alkyl-[NH-C_1-C_4alkylene]$_m$, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17}, or C_6-C_{12}aryl unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18};

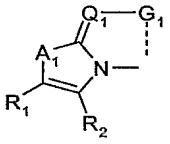
R_{15} is hydrogen, cyano, COO-R_{25} or C_1-C_{12}alkyl;

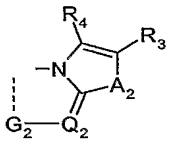
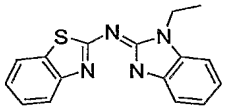
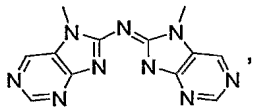
R_{17} is halogen, hydroxy, O-R_{25}, cyano, COO-R_{25} or carboxy; and

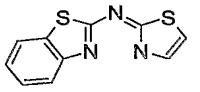
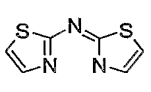
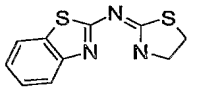
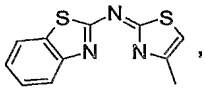
R_{18} is halogen, nitro, cyano, O-R_{19}, $CH=C(CN)_2$, $COOR_{19}$, ureido, $CONR_{25}R_{26}$, SO_2R_{25}, $P(=O)OR_{19}OR_{23}$ or unsubstituted or substituted C_1-C_{12}alkyl.

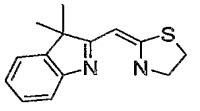
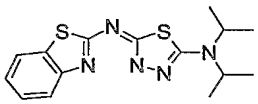
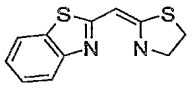
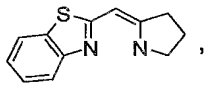
Those preferred meanings apply both individually and in any combination. The compounds of formula (I) generally exhibit more advantageous properties, the more

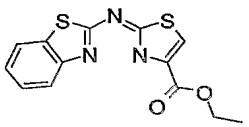
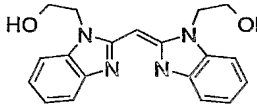
preferred individual features they have.

Also preferred are compounds of formula (I) wherein  and/or

 is/are  ,  ,

 ,  ,  ,  ,

 ,  ,  ,  ,

 or  .

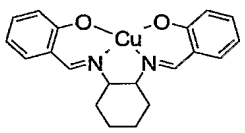
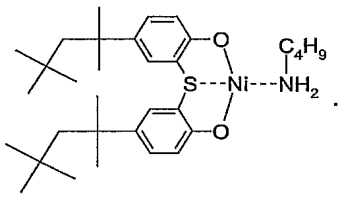
The recording layer advantageously comprises a compound of formula (I) or a mixture of such compounds as main component, for example at least 30 % by weight, preferably at least 60 % by weight, especially at least 80 % by weight. Further customary constituents are possible, for example other chromophores (for example those disclosed in WO 01/75873, or others having an absorption maximum at from 300 to 1000 nm), stabilisers, $^1O_2$-, triplet- or luminescence-quenchers, melting-point reducers, decomposition accelerators or any other additives that have already been described in optical recording media. Preferably, stabilisers or fluoresence-quenchers are added if desired.

When the recording layer comprises further chromophores, the amount of such

chromophores should preferably be small, so that the absorption thereof at the wavelength of the inversion point of the longest-wavelength flank of the absorption of the entire solid layer is a fraction of the absorption of the pure compound of formula (I) in the entire solid layer at the same wavelength, advantageously at most 1/3, preferably at most 1/5, especially at most 1/10. The absorption maximum is preferably higher than 425 nm, especially higher than 500 nm.

Stabilisers, $^1O_2$-, triplet- or luminescence-quenchers are, for example, metal complexes of N- or S-containing enolates, phenolates, bisphenolates, thiolates or bisthiolates or of azo, azomethine or formazan dyes, such as bis(4-dimethylamino-dithiobenzil)nickel [CAS N° 38465-55-3], ®Irgalan Bordeaux EL, ®Cibafast N or similar compounds, hindered phenols and derivatives thereof (optionally also as counter-ions X), such as ®Cibafast AO, o-hydroxyphenyl-triazoles or -triazines or other UV absorbers, such as ®Cibafast W or ®Cibafast P or hindered amines (TEMPO or HALS, also as nitroxides or NOR-HALS, optionally also as counter-ions X), and also as cations diimmonium, Paraquat™ or Orthoquat™ salts, such as ®Kayasorb IRG 022, ®Kayasorb IRG 040, optionally also as radical ions, such as N,N,N',N'-tetrakis(4-dibutylaminophenyl)-p-phenyleneamine-ammonium hexafluorophosphate, hexafluoroantimonate or perchlorate. The latter are available from Organica (Wolfen / DE); ®Kayasorb brands are available from Nippon Kayaku Co. Ltd., and ®Irgalan and ®Cibafast brands are available from Ciba Spezialitätenchemie AG.

Many such structures are known, some of them also in connection with optical recording media, for example from US-5 219 707, JP-A-06/199045, JP-A-07/76169, JP-A-07/262604 or JP-A-2000/272241. They may be, for example, salts of the metal complex anions disclosed above with any desired cations, for example the cations disclosed above, or metal complexes, illustrated, for example, by a compound of

formula  or  .

The person skilled in the art will know from other optical information media, or will easily identify, which additives in which concentration are particularly well suited to which purpose. Suitable concentrations of additives are, for example, from 0.001 to 1000% by weight, preferably from 1 to 50% by weight, based on the recording medium of formula (I).

The optical recording materials according to the invention exhibit excellent spectral properties of the solid amorphous recording layer. The refractive index is extraordinarily high, in some cases even above 2.5. By virtue of an aggregation tendency in the solid that is surprisingly low for such compounds, the absorption band is narrow and intense, the absorption band being especially steep on the long-wavelength side. Crystallites are unexpectedly and very advantageously not formed or are formed only to a negligible extent. The reflectivity of the layers in the range of the writing and reading wavelength is very high in the unwritten state.

By virtue of those excellent layer properties it is possible to obtain a rapid optical recording having high sensitivity, high reproducibility and geometrically very precise mark boundaries, the refractive index and the reflectivity changing substantially, which gives a high degree of contrast. The differences in the mark lengths and the interval distances ("jitter") are very small, which enables a high storage density to be obtained using a relatively thin recording channel with a narrow track spacing ("pitch"). In addition, the recorded data are played back with an astonishingly low error rate, so that error correction requires only a small amount of storage space.

By virtue of the excellent solubility, including in apolar solvents, solutions can be

used even in high concentrations without troublesome precipitation, for example during storage, so that problems during spin-coating are largely eliminated. This applies especially to compounds containing branched C_3-C_8alkyl.

Recording and playback can take place at the same wavelength, therefore advantageously requiring a simple optical system with a single laser source of advantageously from 350 to 500 nm, preferably from 370 to 450 nm. Especially preferred is the UV range from 370 to 390 nm, especially approximately 380 nm, or especially at the edge of the visible range of from 390 to 430 nm, more especially approximately 405 ± 5 nm. In the field of compact, blue or violet laser diodes (such as Nichia GaN 405 nm) with an optical system of high numerical aperture the marks can be so small and the tracks so narrow that up to about 20 to 25 Gb per recording layer is achievable on a 120 mm disc. At 380 nm it is possible to use indium-doped UV-VCSELs (Vertical-Cavity Surface-Emitting Laser), which laser source already exists as a prototype [Jung Han *et al.*, see MRS Internet J. Nitride Semicond. Res. 5S1, W6.2 (2000)].

The invention therefore relates also to a method of recording or playing back data, wherein the data on an optical recording medium according to the invention are recorded or played back at a wavelength of from 350 to 500 nm.

The recording medium is based on the structure of known recording media and is, for example, analogous to those mentioned above. It may be composed, for example, of a transparent substrate, a recording layer comprising at least one of the compounds of formula (I), a reflector layer and a covering layer, the writing and readout being effected through the substrate.

Suitable substrates are, for example, glass, minerals, ceramics and thermosetting and thermoplastic plastics. Preferred supports are glass and homo- or co-polymeric plastics. Suitable plastics are, for example, thermoplastic polycarbonates, polyamides, polyesters, polyacrylates and polymethacrylates, polyurethanes, polyolefins, polyvinyl chloride, polyvinylidene fluoride, polyimides, thermosetting polyesters and

epoxy resins. Special preference is given to polycarbonate substrates which can be produced, for example, by injection-moulding. The substrate can be in pure form or may comprise customary additives, for example UV absorbers or dyes, as proposed e.g. in JP-A-04/167239 as light stabilisation for the recording layer. In the latter case it may be that in the range of the writing wavelength (emission wavelength of the laser) the dye added to the support substrate has no or at most only very low absorption, preferably up to a maximum of about 20% of the laser light focussed onto the recording layer.

The substrate is advantageously transparent over at least a portion of the range from 350 to 500 nm, so that it is permeable to, for example, at least 80 % of the incident light of the writing or readout wavelength. The substrate is advantageously from 10 μm to 2 mm thick, preferably from 100 to 1200 μm thick, especially from 600 to 1100 μm thick, with a preferably spiral guide groove (track) on the coating side, a groove depth of from 10 to 200 nm, preferably from 80 to 150 nm, a groove width of from 100 to 400 nm, preferably from 150 to 250 nm, and a spacing between two turns of from 200 to 600 nm, preferably from 350 to 450 nm. Grooves of different cross-sectional shape are known, for example rectangular, trapezoidal or V-shaped. Analogously to the known CD-R and DVD-R media, the guide groove may additionally undergo a small periodic or quasi-periodic lateral deflection (wobble), so that synchronisation of the speed of rotation and the absolute positioning of the reading head (pick-up) are made possible. Instead of, or in addition to, the deflection, the same function can be performed by markings between adjacent grooves (pre-pits).

The recording medium is applied, for example, by application of a solution by spin-coating, the objective being to produce a layer that is as amorphous as possible, the thickness of which layer is advantageously from 0 to 40 nm, preferably from 1 to 20 nm, especially from 2 to 10 nm, on the surface ("land") and, depending upon the geometry of the groove, advantageously from 20 to 150 nm, preferably from 50 to 120 nm, especially from 60 to 100 nm, in the groove.

Reflecting materials suitable for the reflector layer include especially metals, which provide good reflection of the laser radiation used for recording and playback, for example the metals of Main Groups III, IV and V and of the Sub-Groups of the Periodic Table of the Elements. Al, In, Sn, Pb, Sb, Bi, Cu, Ag, Au, Zn, Cd, Hg, Sc, Y, La, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, Pt and the lanthanide metals Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu and alloys thereof are especially suitable. On account of its high reflectivity and ease of production special preference is given to a reflective layer of aluminium, silver, gold or an alloy thereof (for example a white gold alloy), especially aluminium on economic and ecological grounds. The reflector layer is advantageously from 5 to 200 nm thick, preferably from 10 to 100 nm thick, especially from 40 to 60 nm thick, but reflector layers of greater thickness, for example 1 mm thick or even more, are also possible.

Materials suitable for the covering layer include chiefly plastics, which are applied in a thin layer to the reflector layer either directly or with the aid of adhesion promoters. It is advantageous to select mechanically and thermally stable plastics having good surface properties, which can be modified further, for example written on. The plastics may be thermosetting plastics and thermoplastic plastics. Directly applied covering layers are preferably radiation-cured (e.g. using UV radiation) coatings, which are particularly simple and economical to produce. A wide variety of radiation-curable materials are known. Examples of radiation-curable monomers and oligomers are acrylates and methacrylates of diols, triols and tetrols, polyimides of aromatic tetracarboxylic acids and aromatic diamines having C_1-C_4alkyl groups in at least two ortho-positions of the amino groups, and oligomers with dialkylmaleinimidyl groups, e.g. dimethylmaleinimidyl groups. For covering layers that are applied using adhesion promoters it is preferable to use the same materials as those used for the substrate layer, especially polycarbonates. The adhesion promoters used are preferably likewise radiation-curable monomers and oligomers. Instead of the covering layer applied using an adhesion promoter there may also be used a second substrate comprising a recording and reflector layer, so that the recording medium is

playable on both sides. Preference is given to a symmetrical structure, the two parts being joined together at the reflector side by an adhesion promoter directly or by way of an intermediate layer.

In such a structure, the optical properties of the covering layer, or the covering materials, are essentially unimportant *per se* provided that, where applicable, curing thereof e.g. by UV radiation is achieved. The function of the covering layer is to ensure the mechanical strength of the recording medium as a whole and, if necessary, the mechanical strength of thin reflector layers. If the recording medium is sufficiently robust, for example when a thick reflector layer is present, it is even possible to dispense with the covering layer altogether. The thickness of the covering layer depends upon the thickness of the recording medium as a whole, which should preferably be a maximum of about 2 mm thick. The covering layer is preferably from 10 μm to 1 mm thick.

The recording media according to the invention may also have additional layers, for example interference layers or barrier layers. It is also possible to construct recording media having a plurality of (for example from two to ten) recording layers. The structure and the use of such materials are known to the person skilled in the art. Where present, interference layers are preferably arranged between the recording layer and the reflecting layer and/or between the recording layer and the substrate and consist of a dielectric material, for example as described in EP-A-0 353 393 of TiO_2, Si_3N_4, ZnS or silicone resins.

The recording media according to the invention can be produced by processes known *per se*, it being possible for various methods of coating to be employed depending upon the materials used and their function.

Suitable coating methods are, for example, immersion, pouring, brush-coating, blade-application and spin-coating, as well as vapour-deposition methods carried out under a high vacuum. When, for example, pouring methods are used, solutions in organic solvents are generally employed. When solvents are employed, care should

be taken that the supports used are insensitive to those solvents. Suitable coating methods and solvents are described, for example, in EP-A-0 401 791.

The recording layer is applied preferably by the application of a dye solution by spin-coating, solvents that have proved satisfactory being especially alcohols, e.g. 2-methoxyethanol, isopropanol or n-butanol, hydroxyketones, for example diacetone alcohol or 3-hydroxy-3-methyl-2-butanone, hydroxy esters, for example lactic acid methyl ester or isobutyric acid methyl ester, or preferably fluorinated alcohols, for example 2,2,2-trifluoroethanol or 2,2,3,3-tetrafluoro-1-propanol, and mixtures thereof. Further suitable solvents are disclosed, for example, in EP-A-0 483 387.

The application of the metallic reflector layer is preferably effected by sputtering or by vapour-deposition *in vacuo*. Such techniques are known and are described in specialist literature (e.g. J.L. Vossen and W. Kern, "Thin Film Processes", Academic Press, 1978). The operation can advantageously be carried out continuously and achieves good reflectivity and a high degree of adhesiveness of the metallic reflector layer.

Recording is carried out in accordance with known methods by writing pits (marks) of fixed or variable length by means of a modulated, focussed laser beam guided at a constant or variable speed over the surface of the recording layer. Readout of information is carried out according to methods known *per se* by registering the change in reflection using laser radiation, for example as described in "CD-Player und R-DAT Recorder" (Claus Biaesch-Wiepke, Vogel Buchverlag, Würzburg 1992).The person skilled in the art will be familiar with the requirements.

The information-containing medium according to the invention is especially an optical information material of the WORM type. It can be used, for example, analogously to CD-R (compact disc - recordable) or DVD-R (digital video disc – recordable) in computers, and also as storage material for identification and security cards or for the production of diffractive optical elements, for example holograms.

Alternatively, however, there are also recording media which differ substantially from CD-R and DVD-R and in which recording and playback take place not through the substrate but through the covering layer ("in-groove recording"). Accordingly the respective roles of the covering layer and the substrate, especially the geometry and the optical properties, are reversed in comparison with the structure described above. Analogous concepts are described a number of times in Proceedings SPIE-Int. Soc. Opt. Eng. 1999, 3864 for digital video recordings in conjunction with a blue GaN laser diode. For such recording media, which are especially suitable for a high storage density and have correspondingly small marks ("pits"), precise focussing is important, so that the manufacturing process, while essentially analogous, is considerably more awkward.

The compounds of formula (I) according to the invention, however, also meet the increased demands of an inverse layer structure surprisingly well. Preference is therefore given to an inverse layer structure having the layer sequence substrate, reflector layer, recording layer and covering layer. The recording layer is therefore located between the reflector layer and the covering layer. A thin covering layer approximately from 50 to 400 µm in thickness is especially advantageous (typically 100 µm at a numerical aperture of 0.85).

The recording and reflector layers in an inverse layer structure have in principle the same functions as indicated above. As with the groove geometry, they therefore usually have dimensions within the ranges indicated above.

The inverse layer structure requires particularly high standards, which the compounds used according to the invention fulfil astonishingly well, for example when the recording layer is applied to the metallic reflector layer and especially when a covering layer is applied to the recording layer, the covering layer being required to provide the recording layer with adequate protection against rubbing, photo-oxidation, fingerprints, moisture and other environmental effects and advantageously having a thickness in the range of from 0.01 to 0.5 mm, preferably in the range of

from 0.05 to 0.2 mm, especially in the range of from 0.08 to 0.13 mm.

The covering layer preferably consists of a material that exhibits a transmission of 80% or above at the writing or readout wavelength of the laser. Suitable materials for the covering layer include, for example, those materials mentioned above, but especially polycarbonate (such as Pure Ace® or Panlite®, Teijin Ltd), cellulose triacetate (such as Fujitac®, Fuji Photo Film) or polyethylene terephthalate (such as Lumirror®, Toray Industry), special preference being given to polycarbonate. Especially in the case of directly applied covering layers, radiation-cured coatings, such as those already described above, are advantageous, for example SD 347™ (Dainippon Ink).

The covering layer can be applied directly to the solid recording layer by means of a suitable adhesion promoter. In another embodiment, there is applied to the solid recording layer an additional, thin separating layer of a metallic, crosslinked organometallic or preferably dielectric inorganic material, for example in a thickness of from 0.001 to 10 μm, preferably from 0.005 to 1 μm, especially from 0.01 to 0.1 μm, for example from 0.05 to 0.08 μm in the case of dielectric separating layers and from 0.01 to 0.03 μm in the case of metallic separating layers. Separating layers and corresponding methods are disclosed in WO 02/082438, to which reference is expressly made here. If desired, such coatings can be applied, for example, in the same thickness also between the support material and the metallic reflector layer or between the metallic reflector layer and the optical recording layer. This may be advantageous in certain cases, for example when a silver reflector is used in combination with sulfur-containing additives in the recording layer.

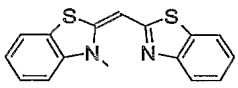
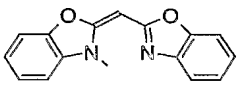
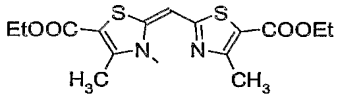
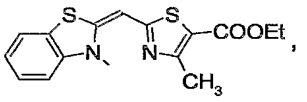
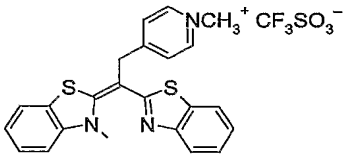
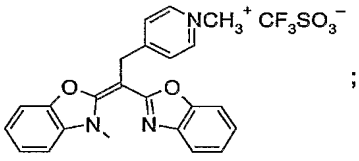
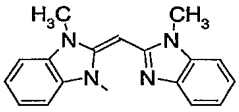
In a special variant, there is applied to the solid recording layer an additional, thin separating layer of a metallic, crosslinked organometallic or dielectric inorganic material, for example in a thickness of from 0.001 to 10 μm, preferably from 0.005 to 1 μm, especially from 0.01 to 0.1 μm. On account of their high reflectivity, metallic separating layers should advantageously be a maximum of 0.03 μm thick.

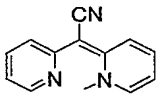
Separating layers and corresponding methods are disclosed in WO 02/082438, to which reference is expressly made here.

Some of the compounds used according to the invention are known, especially from J. Org. Chem. 67/16, 5753-5772 [2002].

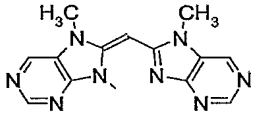
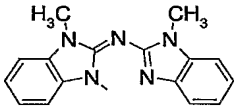
It is also possible, however, to prepare analogously to the known compounds new compounds that can be used in accordance with the invention in optical recording media.

The invention therefore relates also to compounds of formula (I), with the exception of the already known compounds of formula $M_2(Z_1)_2$, wherein:

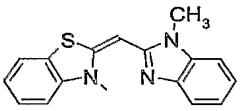
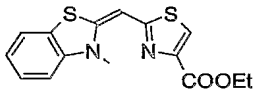
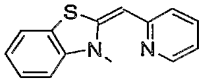
- M_2 is Co(II), Cu(II), Hg(II), Ni(II), Pd(II) or Zn(II) and Z_1 is  ;
- M_2 is Co(II), Cu(II), Ni(II), Pd(II) or Zn(II) and Z_1 is  ,  ,  ,  or  ;
- M_2 is Co(II), Cu(II), Ni(II) or Zn(II) and Z_1 is  ;

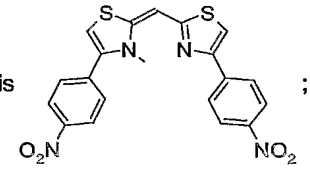
- M_2 is Cu(II), Pd(II) or Zn(II) and Z_1 is  ;

- M_2 is Co(II), Cu(II) or Zn(II) and Z_1 is

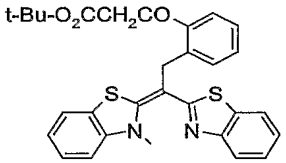
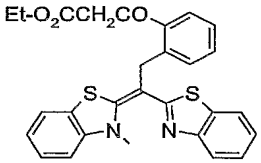
 or  ;

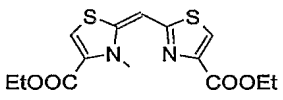
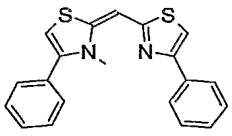
- M_2 is Cu(II) or Zn(II) and Z_1 is

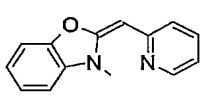
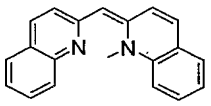
 ,  or  ;

- M_2 is Co(II) or Cu(II) and Z_1 is  ;

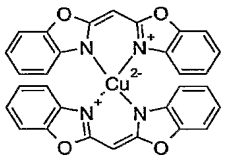
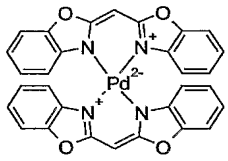
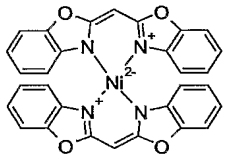
- M_2 is Pd(II) or Zn(II) and Z_1 is

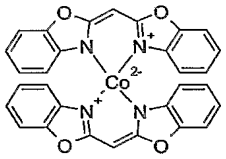
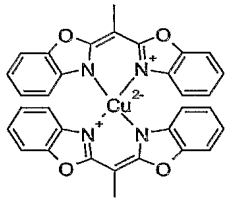
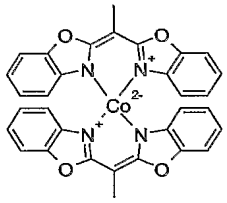
 or  ;

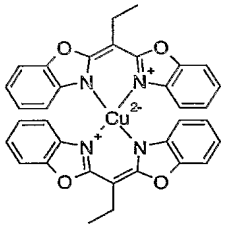
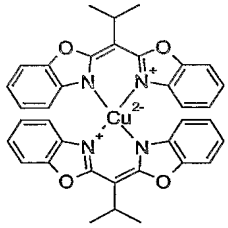
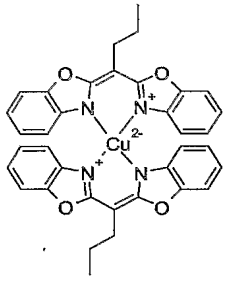
- M_2 is Cu(II) and Z_1 is  or  ; or

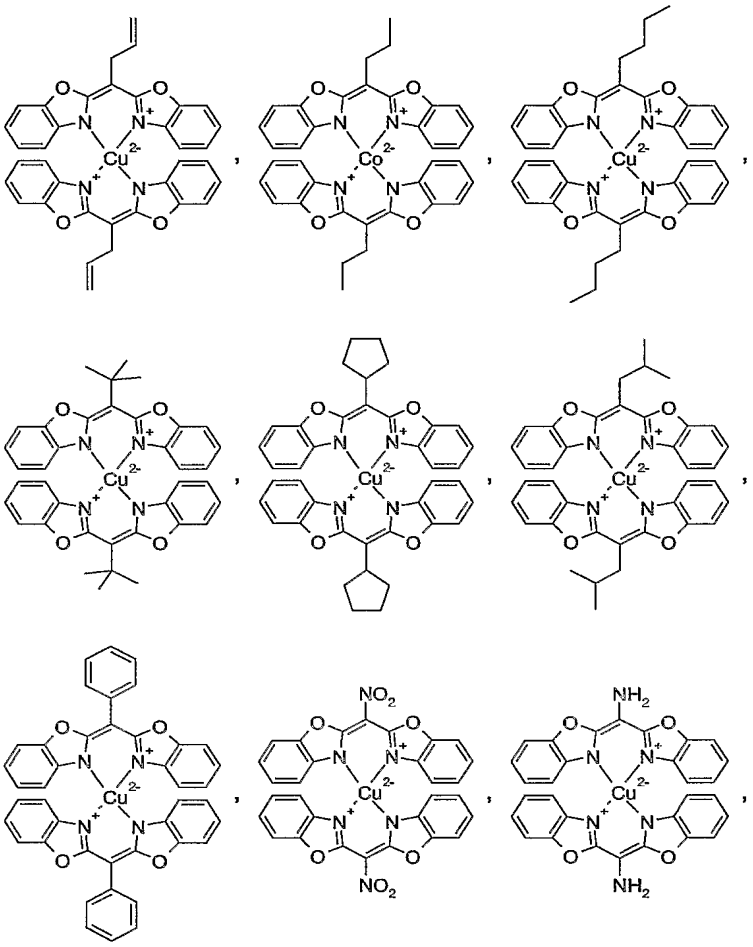
- M_2 is Zn(II) and Z_1 is  or  .

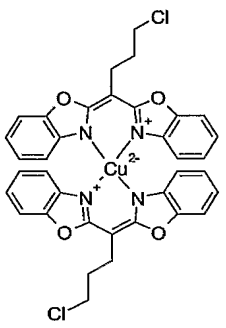
Reference is made especially to compounds of formulae

 ,  ,  ,

 ,  ,  ,

 ,  ,  .

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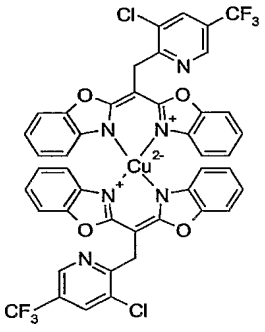
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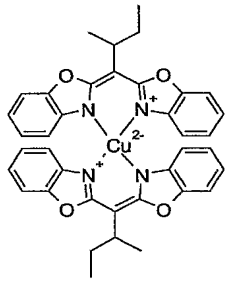
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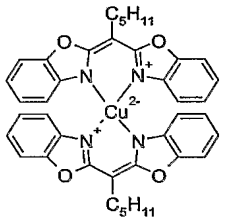
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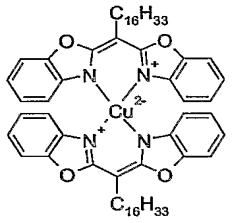
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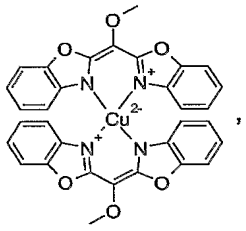
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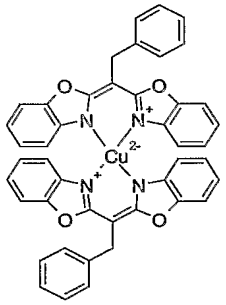
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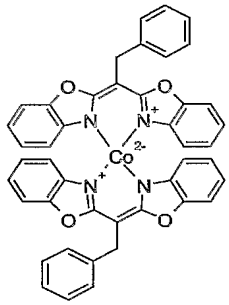
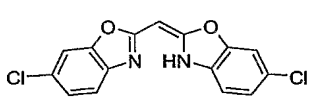

, and to compounds wherein M_2 is

Cu, Co, Ni or Pd and Z_1 is a radical of the following compounds: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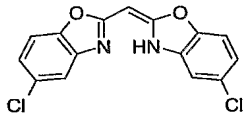
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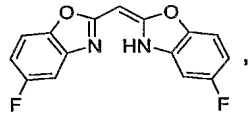
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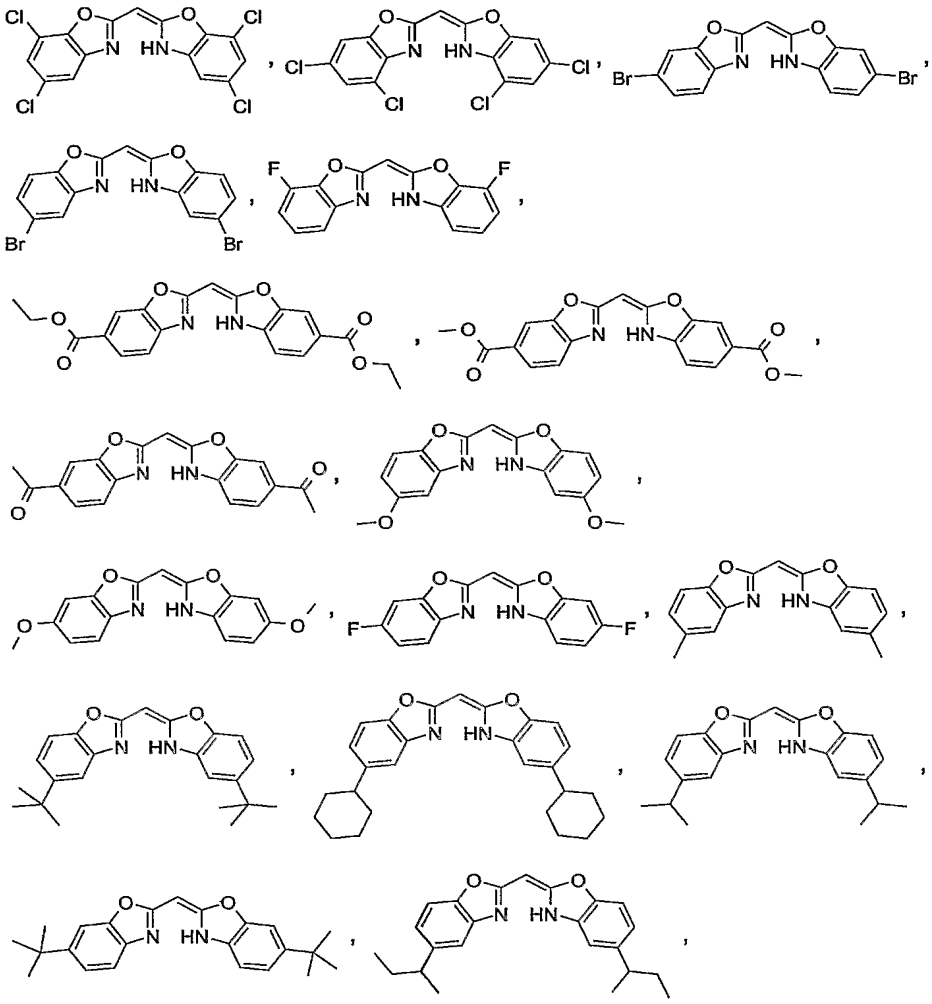
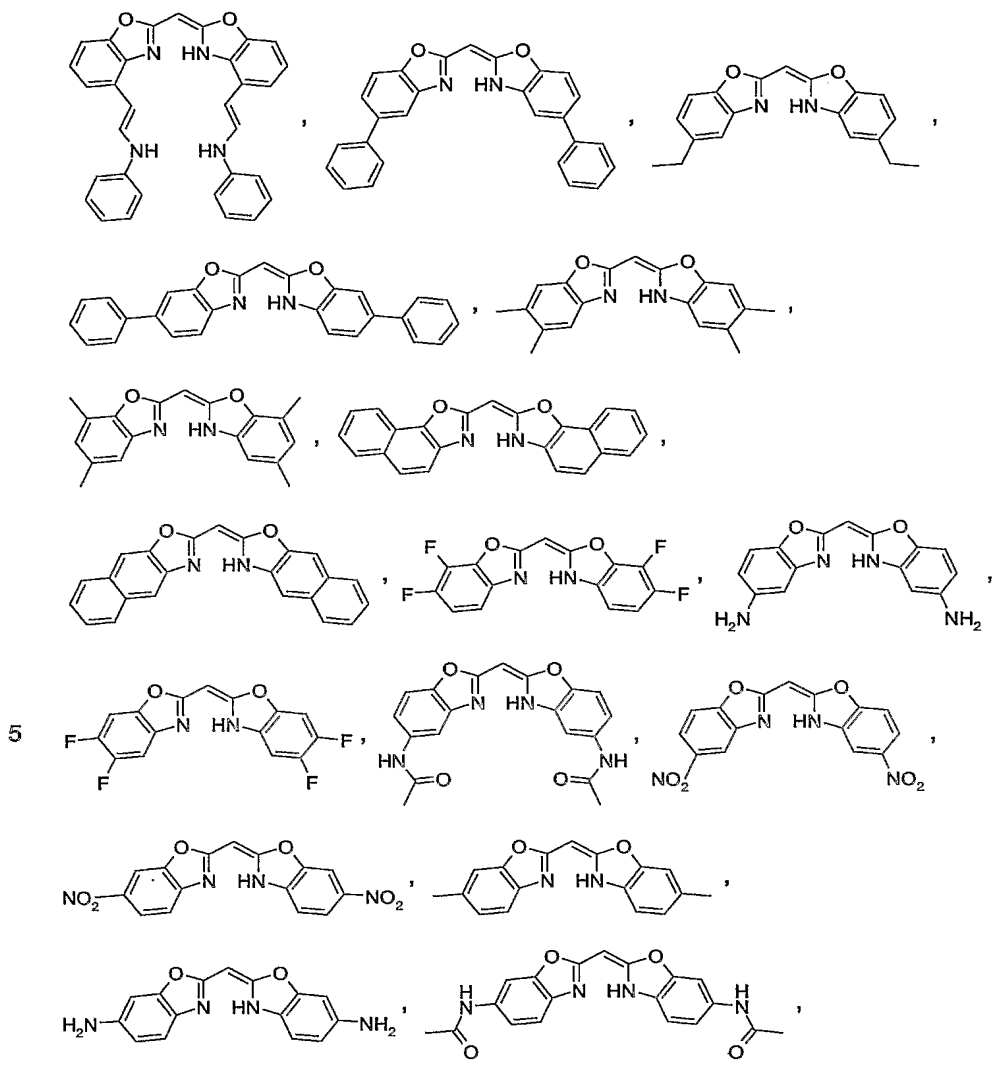
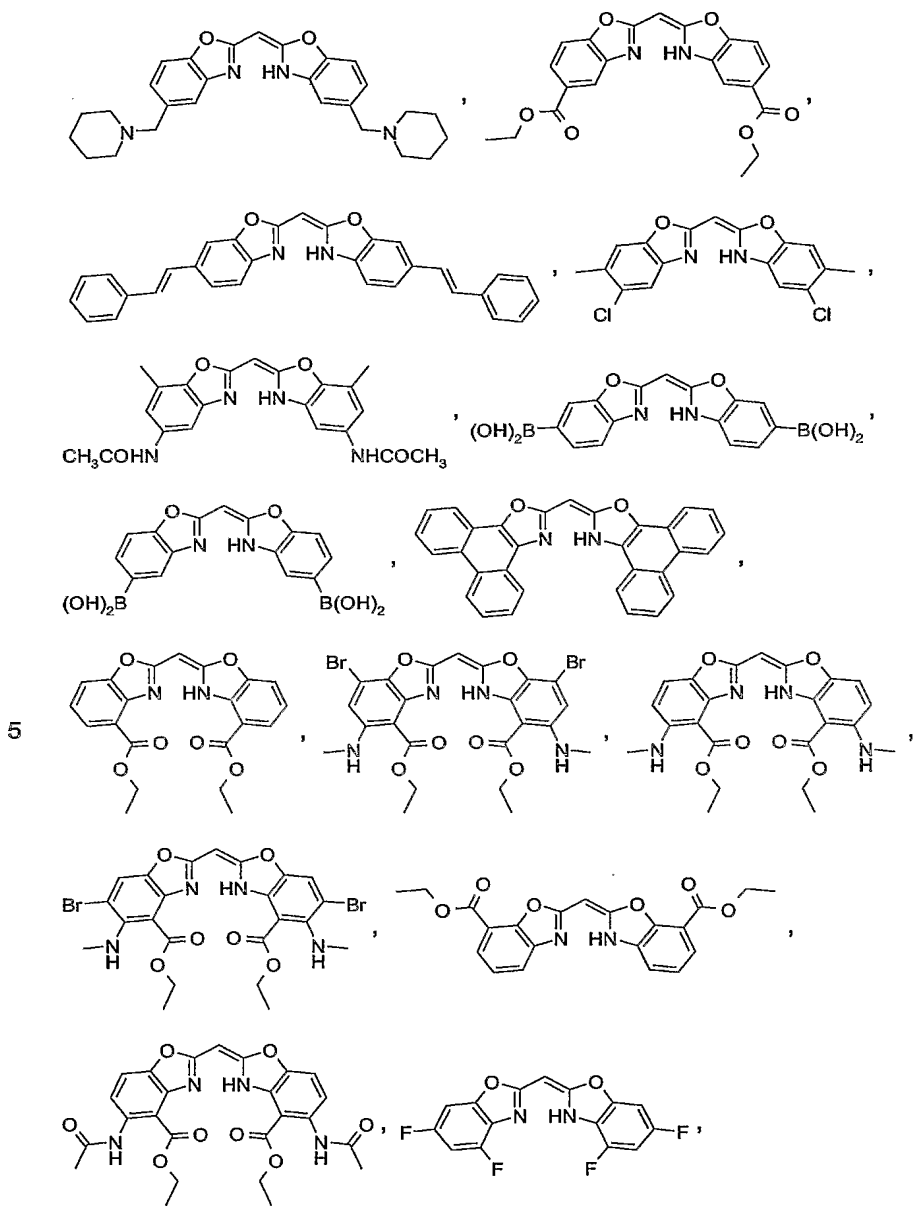
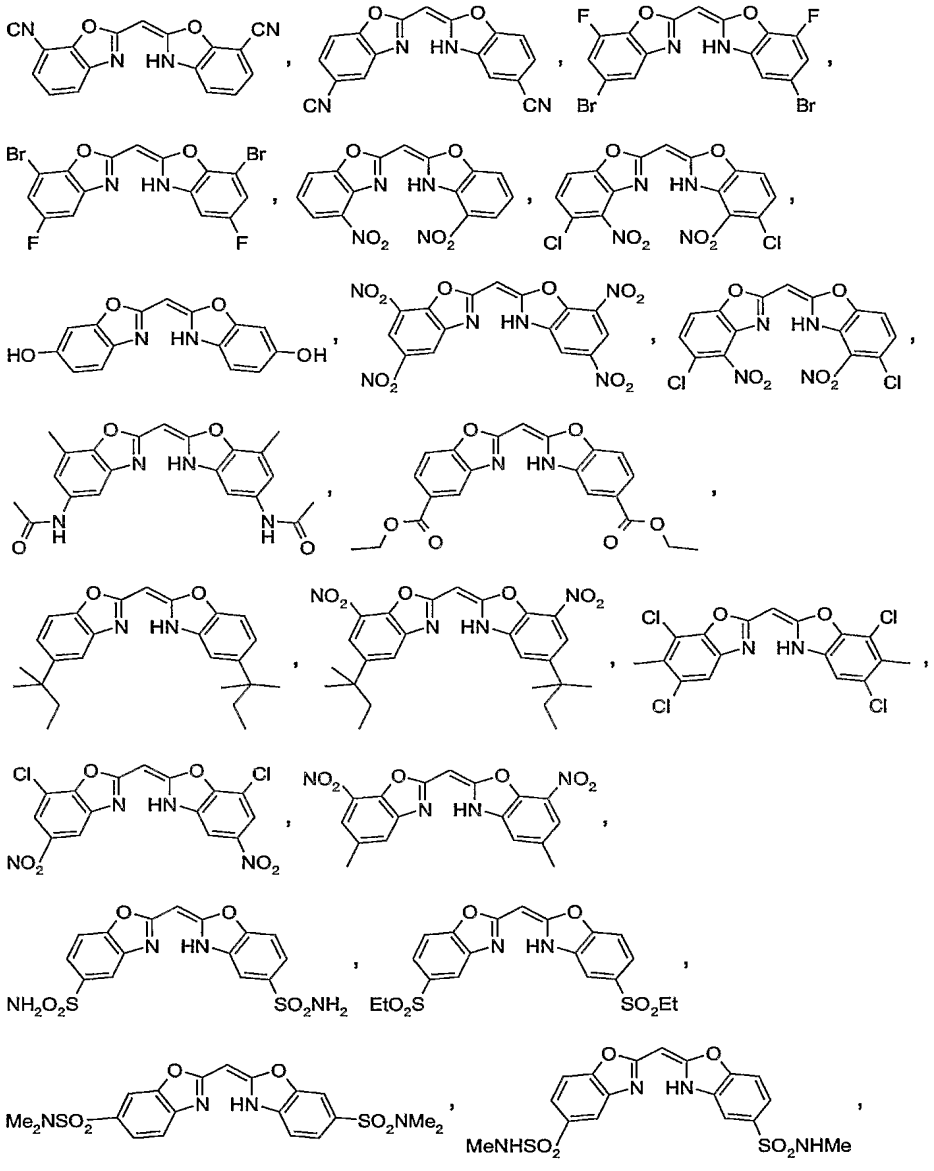
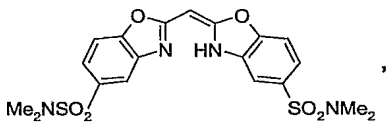


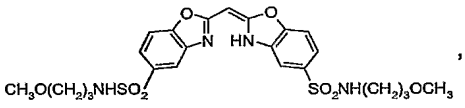







Me2NSO2
SO2NMe2

,


CH3O(CH2)3NHSO2
SO2NH(CH2)3OCH3

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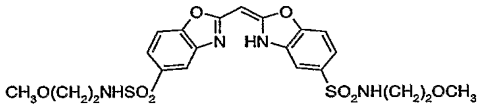
CH3O(CH2)2NHSO2
SO2NH(CH2)2OCH3

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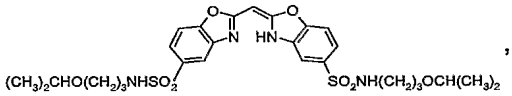
(CH3)2CHO(CH2)3NHSO2
SO2NH(CH2)3OCH(CH3)2

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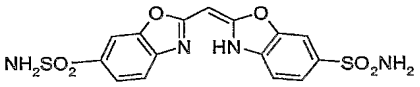
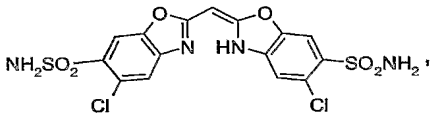
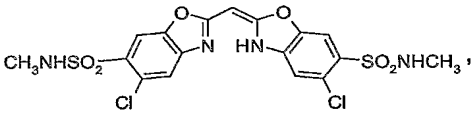

NH2SO2
SO2NH2

,


NH2SO2
SO2NH2
Cl
Cl

,


CH3NHSO2
SO2NHCH3
Cl
Cl

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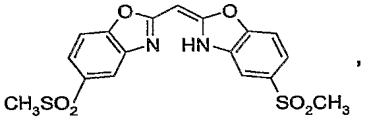
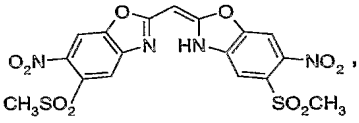
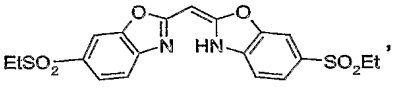

CH3SO2
SO2CH3

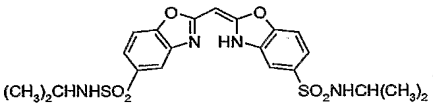
,


O2N
NO2
CH3SO2
SO2CH3

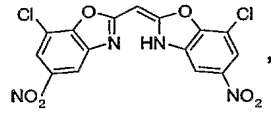
,


EtSO2
SO2Et

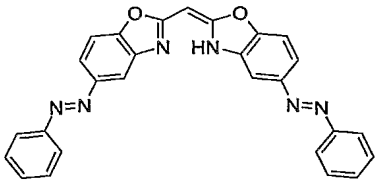
,


(CH3)2CHNHSO2
SO2NHCH(CH3)2

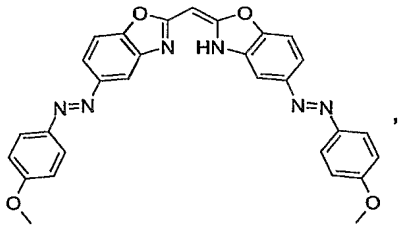
,


Cl
Cl
NO2
NO2

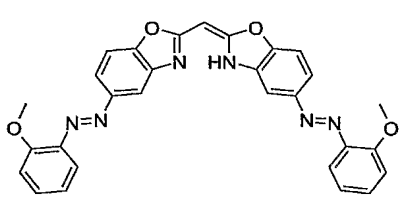
,


N=N
N=N

,


N=N
N=N
O
O

,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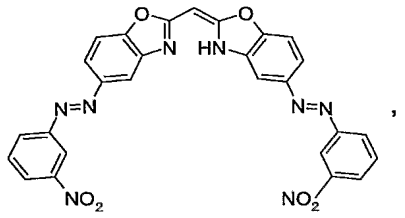
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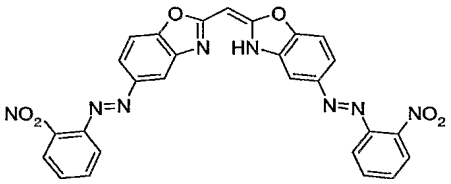
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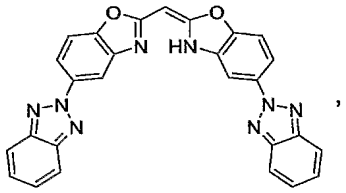
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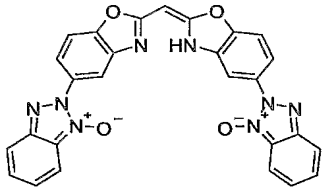
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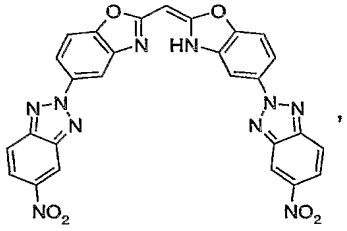
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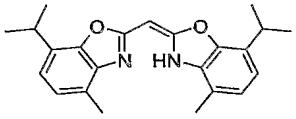
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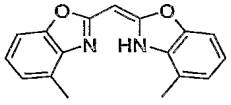
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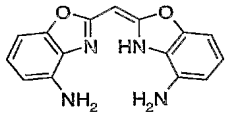
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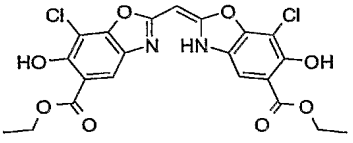
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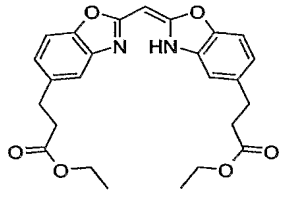
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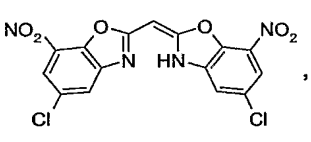
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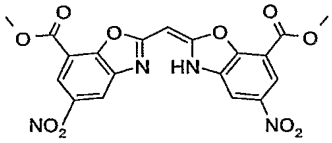
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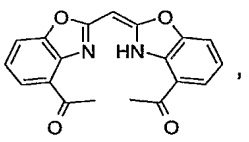
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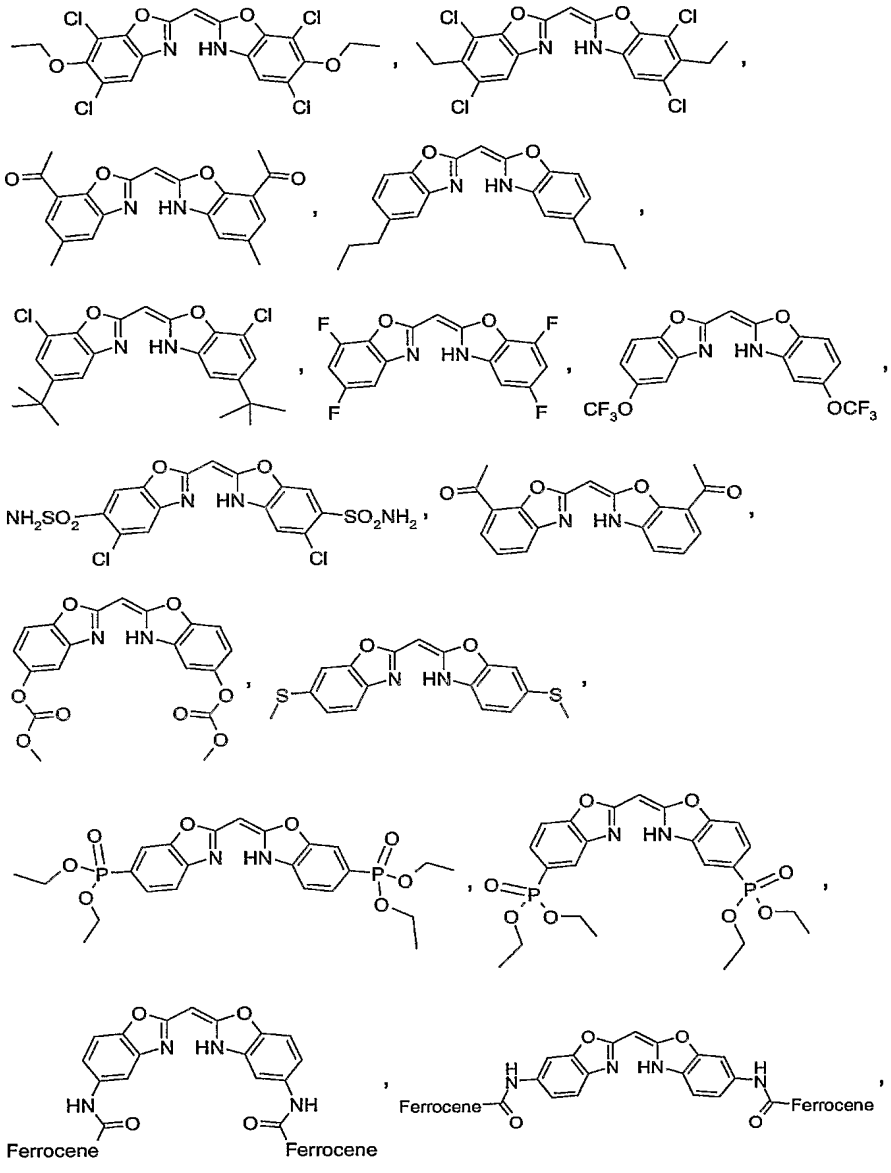
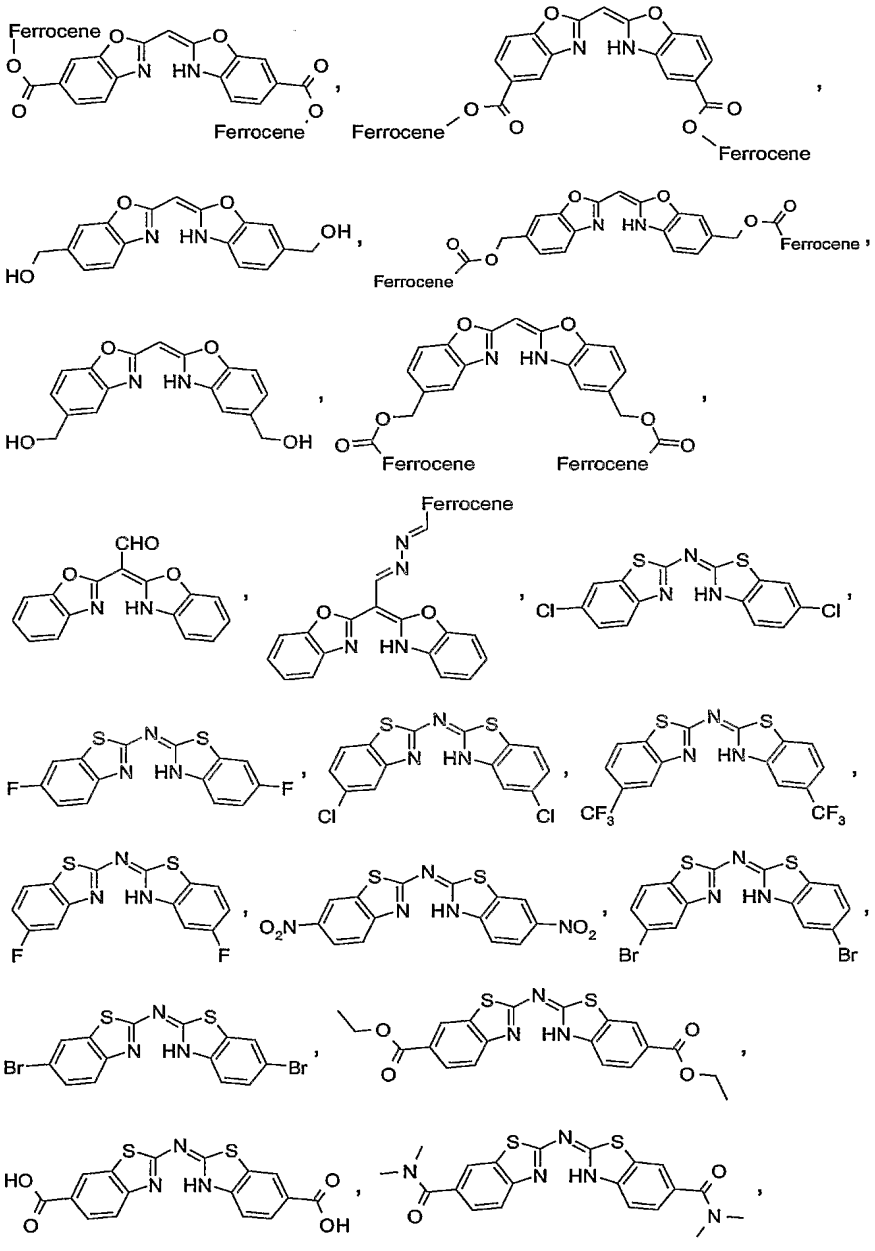
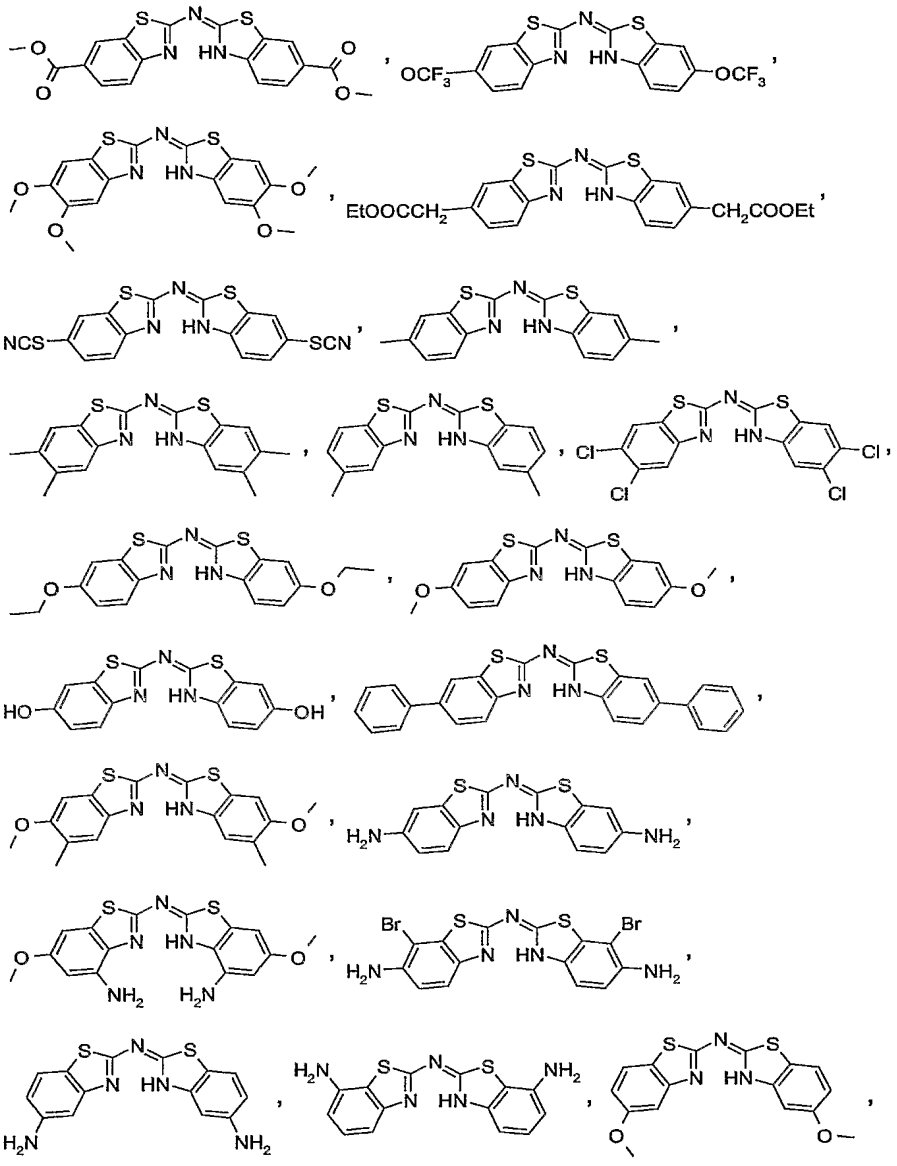
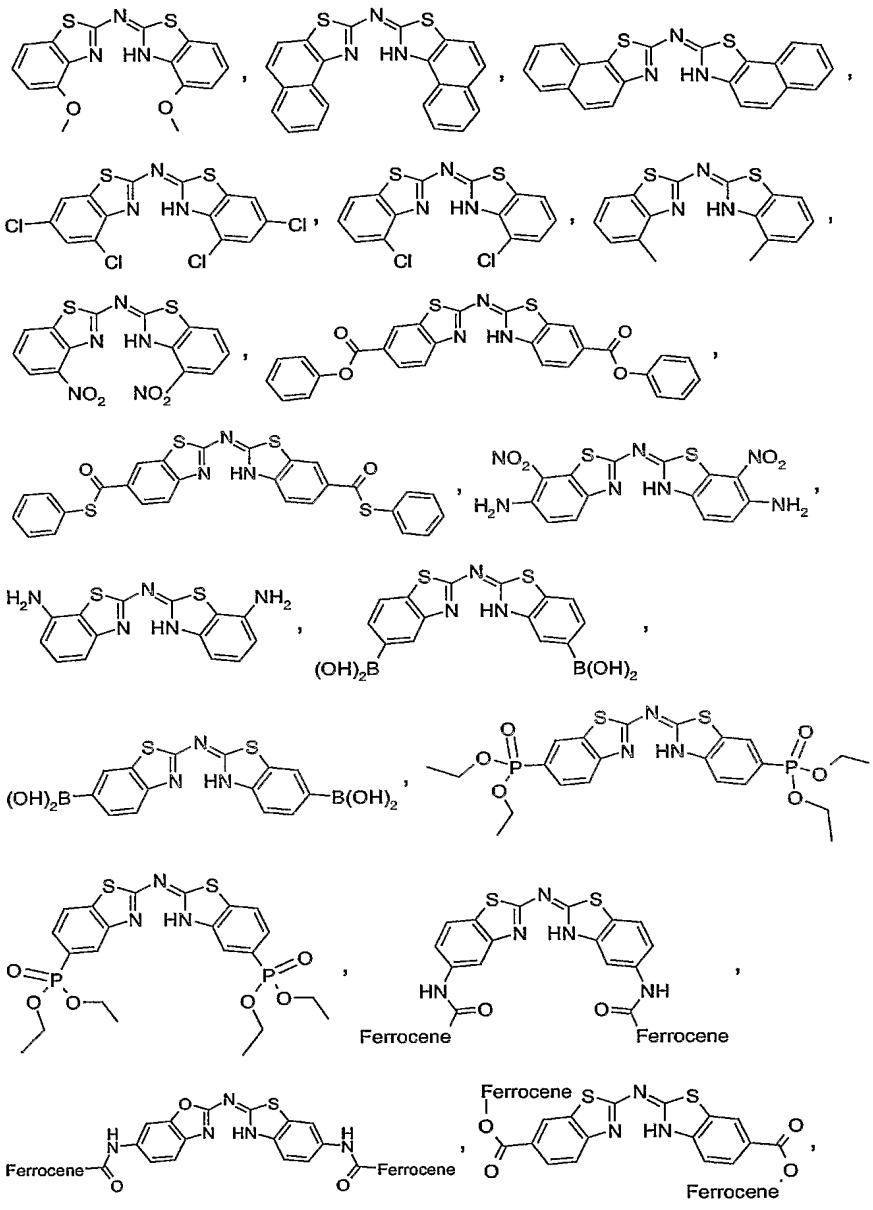
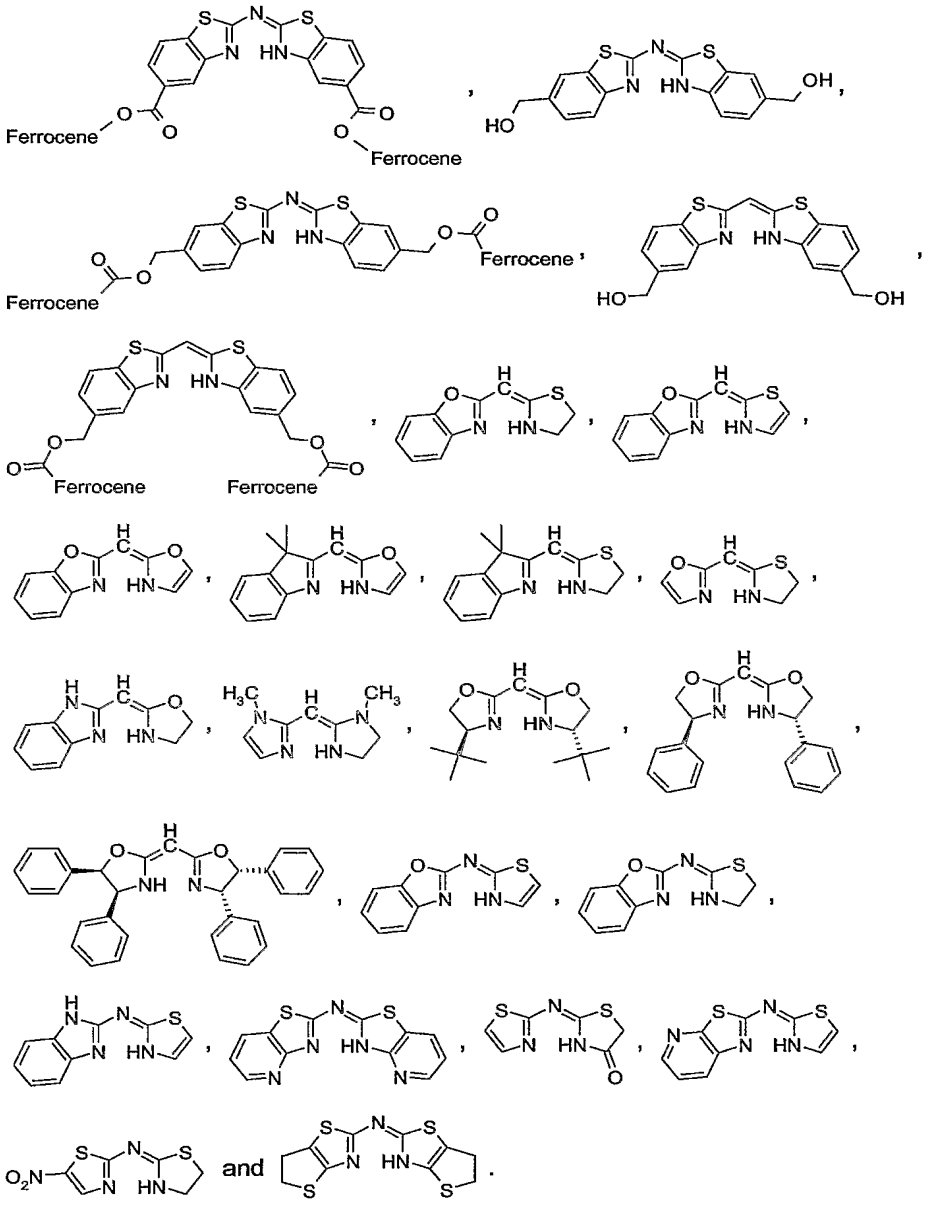


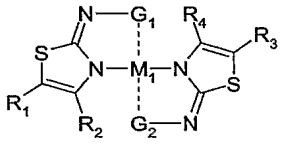
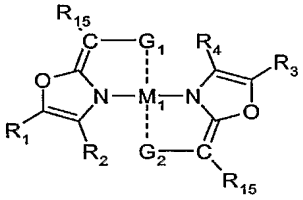






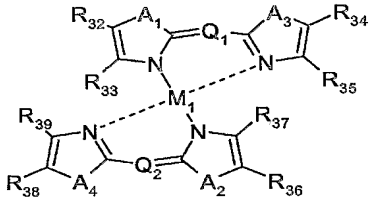


Especially interesting properties are exhibited by the preferred compounds of

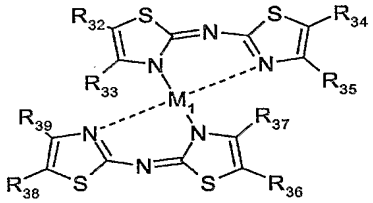
formulae  (II) and  (III) and

also mixtures of compounds of formula (II) and/or (III), wherein especially G_1 and G_2 are the preferred heterocycles disclosed above and at the same time or independently thereof M_1 is a preferred transition metal. A_3 in G_1 and G_2 can be especially $N(R_{12})$, O, S or, especially in formula (III), $C(C_1\text{-}C_5alkyl)_2$.

Special preference is given to compounds of formula

 (IV) and mixtures thereof wherein A_4, independently of A_3, has the same definition and the same preferred meanings as A_3.

Very special preference is given to compounds of formula

 (V).

Both in formula (IV) and in formula (V), R_{32}, R_{33}, R_{34}, R_{35}, R_{36}, R_{37}, R_{38} and R_{39} are preferably H, C_1-C_4alkyl, COO–C_1-C_4alkyl, CN, NO_2, CHO, COC_1-C_4alkyl, phenyl, CH[-O-C_2-C_3alkylene-O-], $C(C_1\text{-}C_4alkyl)$[-O-C_2-C_3alkylene-O-], $CH=C(CN)_2$, $C(CN)=C(CN)_2$ or $C(C_1\text{-}C_4alkyl)=C(CN)_2$, especially H, CH_3, C_2H_5, $COOCH_3$,

$COOC_2H_5$, CN, NO_2 or CHO.

Compounds of formula (IV) are, for example, the following:

Nº	Formula	A_1=A_2	A_3=A_4	Q_1=Q_2	R_{32}=R_{36}	R_{33}=R_{37}	R_{34}=R_{38}	R_{35}=R_{39}	M_1
D1	(IV)	NCH_3	O	N	H	H	H	H	Co^{2+}
D2	(IV)	NCH_2CH_3	O	N	CH_3	H	CH_3	H	Co^{2+}
D3	(IV)	NCH_2CH_3	O	N	CH_3	H	H	H	Co^{2+}
D4	(IV)	S	O	N	NO_2	H	H	H	Co^{2+}
D5	(IV)	S	O	N	NO_2	H	CH_3	H	Co^{2+}
D6	(IV)	NCH_3	NCH_3	N	NO_2	H	NO_2	H	Co^{2+}
D7	(IV)	NCH_2CH_3	NCH_2CH_3	N	CN	H	CN	H	Co^{2+}
D8	(IV)	S	NCH_2CH_3	N	H	H	H	H	Co^{2+}
D9	(IV)	O	O	CH	NO_2	H	NO_2	H	Co^{2+}
D10	(IV)	O	O	CH	CN	H	CN	H	Co^{2+}
D11	(IV)	O	O	CH	SCH_3	H	SCH_3	H	Co^{2+}
D12	(IV)	S	S	N	t-C_4H_9	H	t-C_4H_9	H	Co^{2+}
D13	(IV)	S	S	N	CHO	H	CHO	H	Co^{2+}
D14	(IV)	S	S	N	H	i-C_3H_7	H	i-C_3H_7	Co^{2+}
D15	(IV)	S	S	N	$CHC(CN)_2$	H	$CHC(CN)_2$	H	Co^{2+}
D16	(IV)	NCH_3	O	N	H	H	H	H	Cu^{2+}
D17	(IV)	NCH_2CH_3	O	N	CH_3	H	CH_3	H	Cu^{2+}
D18	(IV)	NCH_2CH_3	O	N	CH_3	H	H	H	Ni^{2+}
D19	(IV)	S	O	N	NO_2	H	H	H	Cu^{2+}
D20	(IV)	S	O	N	NO_2	H	CH_3	H	Cu^{2+}
D21	(IV)	NCH_3	NCH_3	N	NO_2	H	NO_2	H	Ni^{2+}

Nº	Formula	A_1=A_2	A_3=A_4	Q_1=Q_2	R_{32}=R_{36}	R_{33}=R_{37}	R_{34}=R_{38}	R_{35}=R_{39}	M_1
D22	(IV)	NCH_2CH_3	NCH_2CH_3	N	CN	H	CN	H	Cu^{2+}
D23	(IV)	S	NCH_2CH_3	N	H	H	H	H	Cu^{2+}
D24	(IV)	O	O	CH	NO_2	H	NO_2	H	Ni^{2+}
D25	(IV)	O	O	CH	CN	H	CN	H	Cu^{2+}
D26	(IV)	O	O	CH	SCH_3	H	SCH_3	H	Cu^{2+}
D27	(IV)	S	S	N	t-C_4H_9	H	t-C_4H_9	H	Ni^{2+}
D28	(IV)	S	S	N	CHO	H	CHO	H	Cu^{2+}
D29	(IV)	S	S	N	H	i-C_3H_7	H	i-C_3H_7	Cu^{2+}
D30	(IV)	S	S	N	$CHC(CN)_2$	H	$CHC(CN)_2$	H	Ni^{2+}

Compounds of formula (V) are, for example, the following:

Nº	Formula	R_{32}=R_{36}	R_{33}=R_{37}	R_{34}=R_{38}	R_{35}=R_{39}	M_1
D31	(V)	H	H	H	H	Co^{2+}
D32	(V)	CH_3	H	CH_3	H	Co^{2+}
D33	(V)	CH_3	H	H	H	Co^{2+}
D34	(V)	H	CH_3	H	CH_3	Co^{2+}
D35	(V)	H	H	H	CH_3	Co^{2+}
D36	(V)	CH_2CH_3	H	CH_2CH_3	H	Co^{2+}
D37	(V)	CH_2CH_3	H	H	H	Co^{2+}
D38	(V)	n-C_3H_7	H	n-C_3H_7	H	Co^{2+}
D39	(V)	n-C_3H_7	H	H	H	Co^{2+}
D40	(V)	i-C_3H_7	H	i-C_3H_7	H	Co^{2+}
D41	(V)	i-C_3H_7	H	H	H	Co^{2+}

Nº	Formula	R_{32}=R_{36}	R_{33}=R_{37}	R_{34}=R_{38}	R_{35}=R_{39}	M_1
D42	(V)	n-C_4H_9	H	n-C_4H_9	H	Co^{2+}
D43	(V)	n-C_4H_9	H	H	H	Co^{2+}
D44	(V)	i-C_3H_7	CH_3	i-C_3H_7	CH_3	Co^{2+}
D45	(V)	H	H	i-C_3H_7	CH_3	Co^{2+}
D46	(V)	H	i-C_4H_9	H	i-C_4H_9	Co^{2+}
D47	(V)	H	i-C_4H_9	H	H	Co^{2+}
D48	(V)	$COOCH_2CH_3$	CH_3	$COOCH_2CH_3$	CH_3	Co^{2+}
D49	(V)	$COOCH_2CH_3$	CH_3	H	H	Co^{2+}
D50	(V)	H	$COOCH_2CH_3$	H	H	Co^{2+}
D51	(V)	H	$COOCH_2CH_3$	H	$COOCH_2CH_3$	Co^{2+}
D52	(V)	$CH=C(CN)_2$	H	$CH=C(CN)_2$	H	Co^{2+}
D53	(V)	NO_2	H	NO_2	H	Co^{2+}
D54	(V)	H	H	H	H	Cu^{2+}
D55	(V)	CH_3	H	CH_3	H	Cu^{2+}
D56	(V)	CH_3	H	H	H	Cu^{2+}
D57	(V)	H	CH_3	H	CH_3	Cu^{2+}
D58	(V)	H	H	H	CH_3	Cu^{2+}
D59	(V)	CH_2CH_3	H	CH_2CH_3	H	Cu^{2+}
D60	(V)	CH_2CH_3	H	H	H	Cu^{2+}
D61	(V)	n-C_3H_7	H	n-C_3H_7	H	Cu^{2+}
D62	(V)	n-C_3H_7	H	H	H	Cu^{2+}
D63	(V)	i-C_3H_7	H	i-C_3H_7	H	Cu^{2+}
D64	(V)	i-C_3H_7	H	H	H	Cu^{2+}
D65	(V)	n-C_4H_9	H	n-C_4H_9	H	Cu^{2+}

Nº	Formula	R_{32}=R_{36}	R_{33}=R_{37}	R_{34}=R_{38}	R_{35}=R_{39}	M_1
D66	(V)	n-C_4H_9	H	H	H	Cu^{2+}
D67	(V)	i-C_3H_7	CH_3	i-C_3H_7	CH_3	Cu^{2+}
D68	(V)	H	H	i-C_3H_7	CH_3	Cu^{2+}
D69	(V)	H	i-C_4H_9	H	i-C_4H_9	Cu^{2+}
D70	(V)	H	i-C_4H_9	H	H	Cu^{2+}
D71	(V)	$COOCH_2CH_3$	CH_3	$COOCH_2CH_3$	CH_3	Cu^{2+}
D72	(V)	$COOCH_2CH_3$	CH_3	H	H	Cu^{2+}
D73	(V)	H	$COOCH_2CH_3$	H	H	Cu^{2+}
D74	(V)	H	$COOCH_2CH_3$	H	$COOCH_2CH_3$	Cu^{2+}
D75	(V)	$CH=C(CN)_2$	H	$CH=C(CN)_2$	H	Cu^{2+}
D76	(V)	NO_2	H	NO_2	H	Cu^{2+}
D77	(V)	H	H	H	H	Ni^{2+}
D78	(V)	CH_3	H	CH_3	H	Ni^{2+}
D79	(V)	CH_3	H	H	H	Ni^{2+}
D80	(V)	H	CH_3	H	CH_3	Ni^{2+}
D81	(V)	H	H	H	CH_3	Ni^{2+}
D82	(V)	CH_2CH_3	H	CH_2CH_3	H	Ni^{2+}
D83	(V)	CH_2CH_3	H	H	H	Ni^{2+}
D84	(V)	n-C_3H_7	H	n-C_3H_7	H	Ni^{2+}
D85	(V)	n-C_3H_7	H	H	H	Ni^{2+}
D86	(V)	i-C_3H_7	H	i-C_3H_7	H	Ni^{2+}
D87	(V)	i-C_3H_7	H	H	H	Ni^{2+}
D88	(V)	n-C_4H_9	H	n-C_4H_9	H	Ni^{2+}
D89	(V)	n-C_4H_9	H	H	H	Ni^{2+}

Nº	Formula	R_{32}=R_{36}	R_{33}=R_{37}	R_{34}=R_{38}	R_{35}=R_{39}	M_1
D90	(V)	i-C_3H_7	CH_3	i-C_3H_7	CH_3	Ni^{2+}
D91	(V)	H	H	i-C_3H_7	CH_3	Ni^{2+}
D92	(V)	H	i-C_4H_9	H	i-C_4H_9	Ni^{2+}
D93	(V)	H	i-C_4H_9	H	H	Ni^{2+}
D94	(V)	$COOCH_2CH_3$	CH_3	$COOCH_2CH_3$	CH_3	Ni^{2+}
D95	(V)	$COOCH_2CH_3$	CH_3	H	H	Ni^{2+}
D96	(V)	H	$COOCH_2CH_3$	H	H	Ni^{2+}
D97	(V)	H	$COOCH_2CH_3$	H	$COOCH_2CH_3$	Ni^{2+}
D98	(V)	$CH=C(CN)_2$	H	$CH=C(CN)_2$	H	Ni^{2+}
D99	(V)	NO_2	H	NO_2	H	Ni^{2+}

Instead of pure compounds it is also possible to use mixtures thereof, for example the following mixtures:

Nº		%		%		%	%	%
M1	D54	80	D77	20				
M2	D32	5	D54	80	D77	15		
M3	D54	80	D55	10	D78	10		
M4	D54	80	D56	15	D79	5		
M5	D54	80	D55	10	D56	10		
M6	D54	80	D56	20				
M7	D54	80	D56	15	D79	5		
M8	D54	90	D57	10				
M9	D54	80	D57	10	D81	10		
M10	D54	80	D58	20				

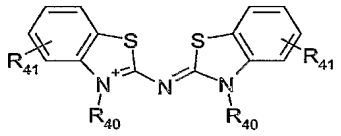
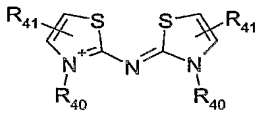
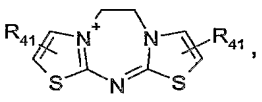
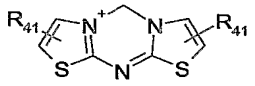
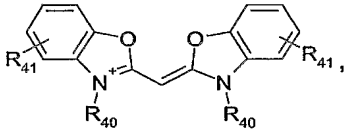
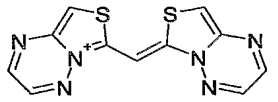
N°		%		%		%		%		%
M11	D54	80	D57	10	D58	10				
M12	D54	65	D57	10	D58	5	D77	15	D81	5
M13	D54	90	D59	10						
M14	D54	80	D60	20						
M15	D54	70	D59	5	D60	10	D76	5	D82	5
M16	D56	90	D61	10						
M17	D56	90	D62	10						
M18	D54	90	D68	10						
M19	D54	90	D71	10						
M20	D54	75	D72	15	D76	5	D95	5		
M21	D54	70	D73	20	D76	5	D96	5		
M22	D54	80	D74	20						
M23	D54	80	D55	5	D56	5	D57	5	D76	5
M24	M5	50	M14	30	D58	5	D76	5	D77	10

Instead of preparing mixtures by mixing together the components, it is favourably possible to prepare mixtures by mixed synthesis, the metals being added in any desired order in succession or preferably simultaneously to a pre-prepared mixture of the ligands, or conversely the ligands being added in any desired order in succession or preferably all of them simultaneously to a pre-prepared mixture of the metals. The mixtures prepared by mixed synthesis generally have somewhat better solubility than physical mixtures, possibly because of their asymmetric components.

In addition to comprising one or more compounds of formula (I) and optionally customary additives, the optical recording media according to the invention may also comprise other chromophores, preferably metal-free chromophores. Other chromophores may, if desired, be added in an amount of from 1 to 200 % by weight,

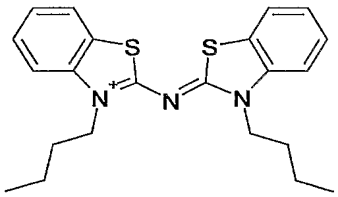
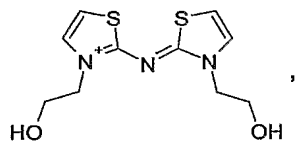
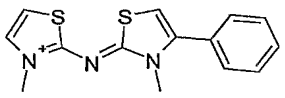
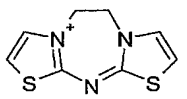
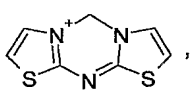
based on the total of the compounds of formula (I). The amount of other chromophores is preferably from 5 to 100 % by weight, especially from 10 to 50 % by weight, based on the total of the compounds of formula (I). Chromophores can be dyes or UV absorbers, preferably having an absorption maximum of from 350 to 400 nm or at from 600 to 700 nm, for example around 380 or 630 nm.

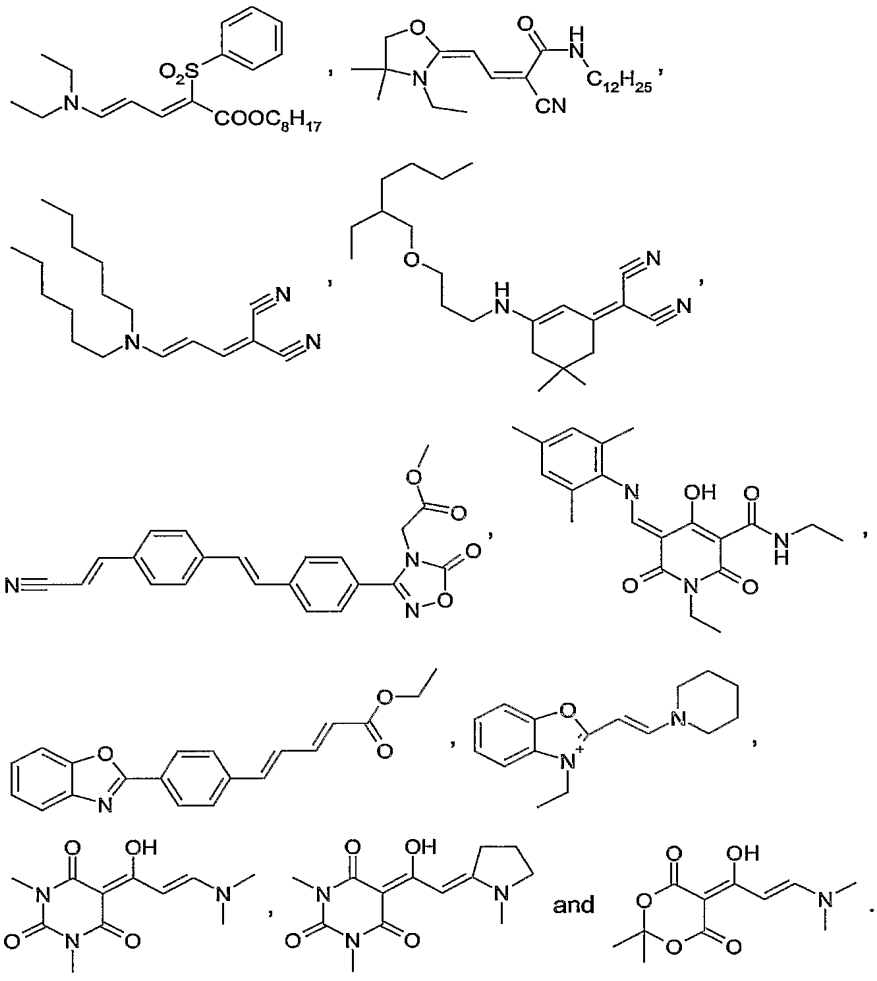
Especially preferred additional metal-free chromophores are cyanines, azacyanines, merocyanines and oxonols and also rhodamines, for example those disclosed in WO 04/006878, WO 02/082438 or EP-A-1 083 555, and also

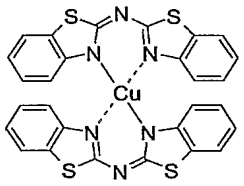
wherein R_{40} is C_1-C_{24}alkyl or C_2-C_{24}alkenyl, each of which can be unsubstituted or substituted, and R_{41} is any substituent. R_{40} may be, for example, methyl, ethyl, vinyl, allyl, isopropyl, n-butyl, 2-isopropyloxy-ethyl, n-pentyl, 3-methyl-butyl, 3,3-dimethyl-butyl, 2-ethyl-hexyl, 2-cyano-ethyl, furan-2-yl-methyl or 2-hydroxy-methyl; R_{41} is, for example, C_6-C_{10}aryl, C_1-C_{24}alkyl or C_2-C_{24}alkenyl.

Purely illustrative examples of such chromophores are:

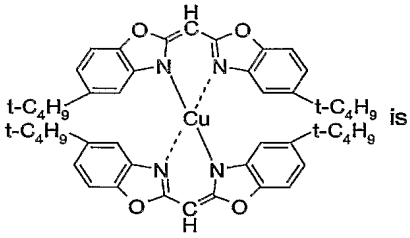


The following Examples illustrate the invention but do not limit the scope thereof (unless otherwise indicated,"%" always refers to % by weight):

Example 1: 1.0 g of the compound of formula  is applied in the form of a dichloromethane solution to glass. The solid layer is irradiated for 90 hours with xenon light according to ISO-105-B02 (Atlas Ci-35 Weather-O-meter, 15 kJ/cm^2). The light stability is excellent (see Example 7).

Example 2: On the solid layer according to Example 1, marks are written into the recording layer using a pulsed dye laser (15 ns pulse length) at a wavelength of 405 nm at an energy density of 0.8 kJ/m^2. The written sites exhibit a resulting change in reflectivity.

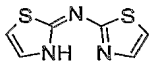
Example 3: 0.5 g of the compound according to Example 1 is dissolved in 99.5 g of dioxane and applied by means of spin-coating to a silicon wafer. The colourless solid layer is measured using a spectral ellipsometer (Sopra). At a wavelength of 405 nm a refractive index of 2.52 is determined.

Example 4: 1.0 g of the compound of formula  is dissolved in 99 g of methylcyclohexane and filtered through a 0.2 µm Teflon filter. The dye solution is then applied by rotation at 250 rev/min to a 1.2 mm thick, flat polycarbonate plate (diameter 120 mm). The rotational speed is then increased to 1200 rev/min, so that the excess solution is spun off, and a uniform solid layer is formed. After drying, the solid layer has an absorption of 0.61 at 382 nm. Using an optical measuring system (ETA-RT, STEAG ETA-Optik), the layer thickness and the

complex refractive index are determined. At 405 nm the dye layer has a layer thickness of 56 nm, a refractive index n of 1.95 and an extinction coefficient k of 0.090.

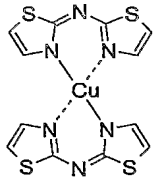
Example 5:

Synthesis of the ligand

19.4 ml of a 55 % aqueous chloracetaldehyde solution are added to a suspension of 10.2 g of dithiobiuret in 45 ml of ethanol. The reaction mixture is heated at 75°C for 2 hours, and then poured into 150 ml of water. After the addition of 200 ml of an aqueous sodium acetate solution (4.6N), the precipitate is filtered off, washed with water and dried at 50°C/1.5 · 10^3 Pa, yielding 8.8 g of crude product, and after recrystallisation from ethanol 6.7 g of pure product of formula 

(m.p. 212°C).

Synthesis of the complex

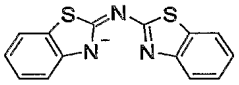
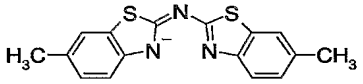
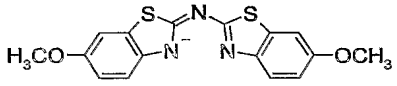
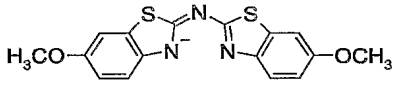
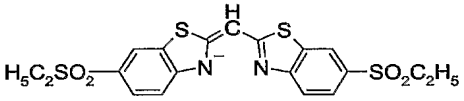
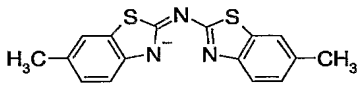
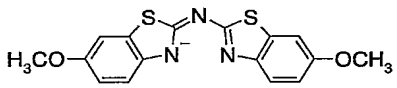
0.5N aqueous copper(II) acetate solution is added to a solution of 458 mg of the resulting ligand in 30 ml of ethanol until precipitation, which begins immediately, is complete. After filtration, the product is washed with ethanol and diethyl ether, and then dried at 70°C/1.5 · 10^3 Pa. 390 mg of pure product of formula 

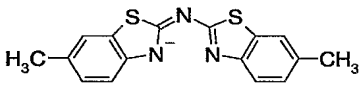
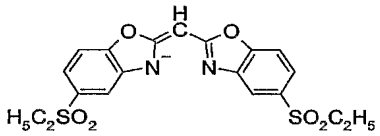
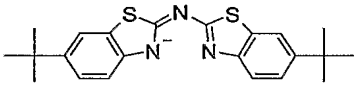
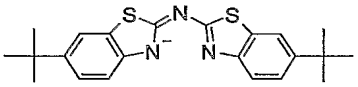
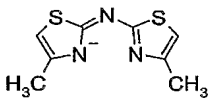
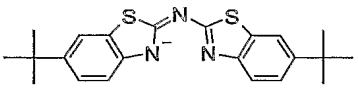
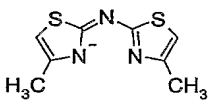
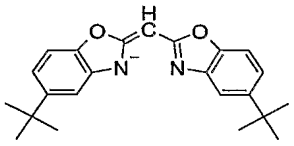
(decomp. 264°C) are obtained.

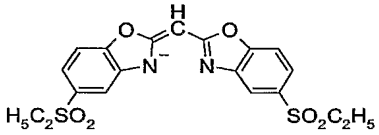
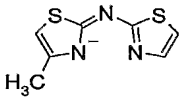
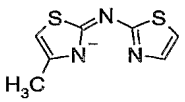
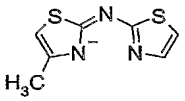
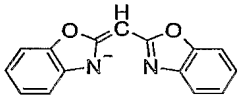
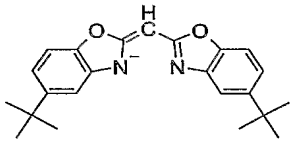
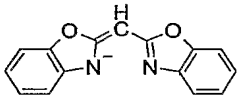
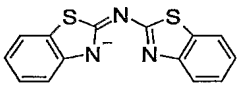
Example 6: 1.0 g of the complex according to Example 5 is dissolved in 99 g of 2,2,3,3-tetrafluoro-1-propanol and filtered through a 0.2 μm Teflon filter. The dye solution is then applied by rotation at 250 rev/min to a 1.2 mm thick, flat polycarbonate plate (diameter 120 mm); the rotational speed is then increased to 1500 rev/min, so that the excess solution is spun off and a uniform solid layer is

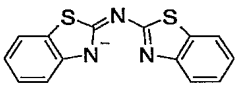
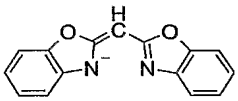
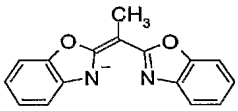
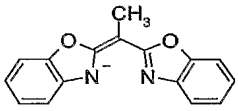
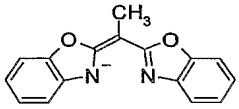
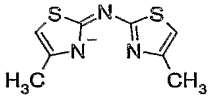
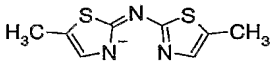
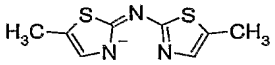
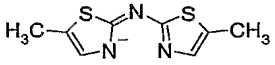
formed. After drying, the solid layer has an absorption of 0.35 at 356 nm. Using an optical measuring system (ETA-RT, STEAG ETA-Optik), the layer thickness and the complex refractive index are determined. At 405 nm the dye layer has a layer thickness of 18 nm, a refractive index n of 2.25 and an extinction coefficient k of 0.031.

Examples 7 – 38: The procedure is analogous to Example 6, but instead of the complex of Example 5 the following ligands and metal cations are used:

Metal	Ligand (2×)	λ_{max} [nm]	Solvent	n	k
Cu^{2+}		370	CH_3CN (+HCl)	2.52	0.47
Cu^{2+}		383	CH_2Cl_2	2.30	0.185
Ni^{2+}		370	CH_2Cl_2	2.23	0.160
Cu^{2+}		390	CH_2Cl_2	2.22	0.266
Cu^{2+}		377	CH_2Cl_2	2.21	0.244
Co^{2+}		370	CH_2Cl_2	2.20	0.137
Co^{2+}		376	CH_2Cl_2	2.19	0.179

Metal	Ligand (2×)	λ_{max} [nm]	Solvent	n	k
Ni^{2+}		361	CH_2Cl_2	2.17	0.108
Co^{2+}		370	CH_2Cl_2	2.08	0.158
Ni^{2+}		361	CH_2Cl_2	2.07	0.097
Cu^{2+}		384	CH_2Cl_2	2.00	0.092
Co^{2+}		351	CH_2Cl_2	1.98	0.100
Co^{2+}		370	CH_2Cl_2	1.94	0.083
Ni^{2+}		350	CH_2Cl_2	1.93	0.083
Co^{2+}		367	CH_2Cl_2	1.83	0.103

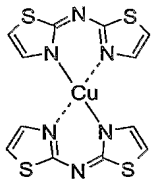
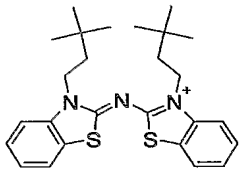
Metal	Ligand (2×)	λ_{max} [nm]	Solvent	n	k
Ni^{2+}		368	CH_2Cl_2	1.74	0.119
Cu^{2+}		369	CH_2Cl_2		
Ni^{2+}		350	CH_2Cl_2		
Co^{2+}		348	CH_2Cl_2		
Ni^{2+}		356	CH_3CN		
Ni^{2+}		357	CH_2Cl_2		
Co^{2+}		364	CH_2Cl_2		
Co^{2+}		370	CH_3CN (+HCl)		

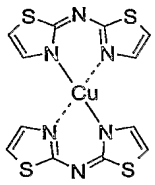
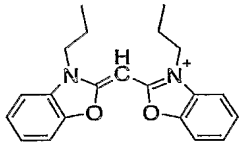
Metal	Ligand (2×)	λ_{max} [nm]	Solvent	n	k
Ni^{2+}		370	CH_3CN (+HCl)		
Cu^{2+}		374	CH_2Cl_2		
Ni^{2+}		374	CH_2Cl_2		
Co^{2+}		376	CH_3CN		
Cu^{2+}		387	CH_2Cl_2		
Cu^{2+}					
Ni^{2+}					
Co^{2+}		350	CH_2Cl_2		
Cu^{2+}		358	CH_2Cl_2		

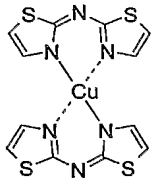
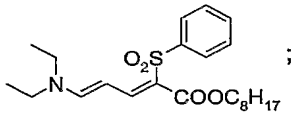
Examples 39 – 62: The procedure is analogous to Example 6, but instead of the complex of Example 5 the mixtures M1 to M24 are used.

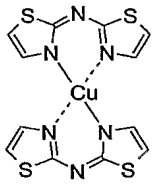
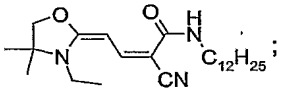
Examples 63 – 86: The procedure is analogous to Example 6, but instead of the complex of Example 5 there are used mixtures having the same proportions of metal and ligand as mixtures M1 to M24 but the complexes are prepared by mixed synthesis (variant of the simultaneous addition of the metal mixture to the ligand mixture). The results are similar to those of Examples 39 – 62, but have surprisingly better solubility and solution stability.

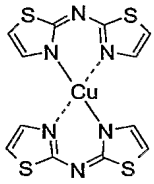
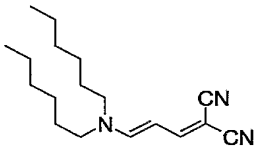
Examples 87 – 94: The procedure is analogous to Example 6, but instead of the complex of Example 5 there are used the following mixtures of compounds of formula (I) with cyanines and merocyanines:

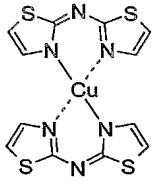
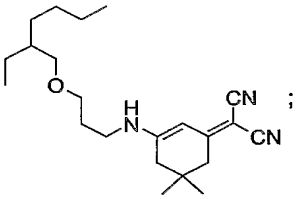
80%  + 20%  ;

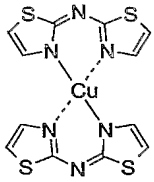
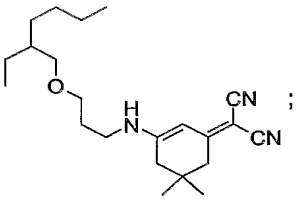
80%  + 20%  ;

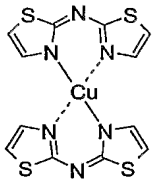
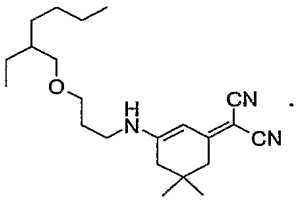
75%  + 25%  ;

75%  + 25%  ;

75%  + 25%  ;

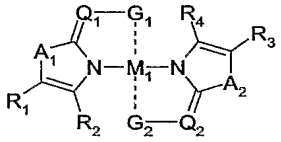
75%  + 25%  ;

50%  + 50%  ;

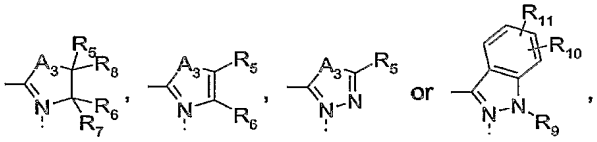
95%  + 5%  .

It will be understood that it is also possible to combine mixtures of those cyanines, merocyanines and/or also other chromophores with complexes of formula (I) or with mixtures of complexes of formula (I), the results achieved generally being very good.

What is claimed is:

1. An optical recording medium comprising a substrate, a recording layer and optionally one or more reflecting layers, wherein the recording layer comprises a compound of formula  (I) or a tautomer thereof, wherein

G_1 and G_2 are each independently of the other



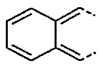
A_1 and A_2 are each independently of the other $N(R_{12})$, O, S or Se and A_3 is $C(C_1\text{-}C_5alkyl)_2$, $C(C_4\text{-}C_5alkylene)$, $N(R_{12})$, O, S, Se, $N{=}C(R_{13})$ or unsubstituted or R_{14}-substituted CH=CH;

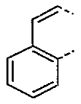
M_1 is a transition metal of groups IX to XII, preferably Co, Cu, Ni, Pd or Zn, especially Co, Cu or Ni;

Q_1 and Q_2 are each independently of the other $C(R_{15})$, N or P;

R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8 and R_{14} are each independently of the others hydrogen, R_{18}, or $C_6\text{-}C_{12}$aryl, $C_4\text{-}C_{12}$heteroaryl, $C_7\text{-}C_{12}$aralkyl or $C_5\text{-}C_{12}$heteroaralkyl each unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18}; or

R_1 and R_2, R_3 and R_4, R_5 and R_6, R_5 and R_{13} and/or R_5 and R_{14}, together in pairs, are $C_3\text{-}C_6$alkylene or $C_3\text{-}C_6$alkenylene, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17} and may be

uninterrupted or interrupted by O, S or N(R_{12}), or 1,4-buta-1,3-dienylene, 

or  , each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18} and in which 1 or 2 carbon atoms may have been replaced by nitrogen;

R_9, R_{12} and R_{13} are each independently of the others C_1-C_{24}alkyl, C_3-C_{24}cycloalkyl, C_2-C_{24}alkenyl, C_3-C_{24}cycloalkenyl, C_1-C_4alkyl-[O-C_1-C_4alkylene]$_m$ or C_1-C_4alkyl-[NH-C_1-C_4alkylene]$_m$, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17}; or C_6-C_{12}aryl, C_4-C_{12}heteroaryl, C_7-C_{12}aralkyl or C_5-C_{12}heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18};

R_{10}, R_{11} and R_{18} are each independently of the others halogen, nitro, cyano, thiocyanato, hydroxy, O-R_{19}, O-CO-R_{19}, S-R_{19}, CHO, COR_{20}, $CHOR_{19}OR_{23}$, $CR_{20}OR_{19}OR_{23}$, R_{16}, N=N-R_{16}, N=$CR_{19}R_{20}$, N=$CR_{21}R_{22}$, C(R_{15})=NR_{19}, C(R_{15})=NR_{21}, C(R_{15})=$CR_{21}R_{22}$, NH_2, NH-R_{19}, $NR_{19}R_{20}$, NH_3^+, $NH_2R_{19}^+$, $NHR_{19}R_{20}^+$, $NR_{19}R_{20}R_{23}^+$, $CONH_2$, $CONHR_{19}$, $CONR_{19}R_{20}$, SO_2R_{19}, SO_2NH_2, SO_2NHR_{19}, $SO_2NR_{19}R_{20}$, COOH, $COOR_{19}$, $OCOOR_{19}$, $NHCOR_{19}$, $NR_{19}COR_{23}$, $NHCOOR_{19}$, $NR_{19}COOR_{23}$, ureido, NR_{19}-CO-NHR_{23}, $B(OH)_2$, B(OH)(OR_{19}), $B(OR_{19})OR_{23}$, phosphato, $PR_{19}R_{23}$, $POR_{19}OR_{23}$, P(=O)$OR_{19}OR_{23}$, $OPR_{19}R_{23}$, $OPR_{19}OR_{23}$, OP(=O)$R_{19}OR_{23}$, OP(=O)$OR_{19}OR_{23}$, OPO_3R_{19}, sulfato, sulfo, or C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_1-C_{12}alkylthio, C_3-C_{12}cycloalkylthio, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy each unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17};

R_{15} is hydrogen, cyano, hydroxy, C_1-C_{12}alkoxy, C_3-C_{12}cycloalkoxy, C_1-C_{12}alkylthio, C_3-C_{12}cycloalkylthio, amino, NHR_{24}, $NR_{25}R_{26}$, R_{27}, halogen, nitro, formyl, N=N-R_{27}, C(R_{14})=$CR_{21}R_{22}$, C(R_{14})=NR_{19}, COO-R_{25}, carboxy, carbamoyl, CONH-R_{25},

$CONR_{25}R_{26}$, $N{=}CR_{19}R_{20}$, or C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_2-C_{12}alkenyl or C_3-C_{12}cycloalkenyl each unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy radicals;

R_{16} is C_6-C_{12}aryl, C_4-C_{12}heteroaryl, C_7-C_{12}aralkyl or C_5-C_{12}heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{28};

R_{17} is halogen, hydroxy, O-R_{25}, O-CO-R_{25}, S-R_{25}, NH_2, NH-R_{25}, $NR_{25}R_{26}$, NH_3^+, $NH_2R_{25}^+$, $NHR_{25}R_{26}^+$, $NR_{24}R_{25}R_{26}^+$, NR_{25}-CO-R_{24}, $NR_{25}COOR_{24}$, cyano, formyl, COO-R_{25}, carboxy, carbamoyl, CONH-R_{25}, $CONR_{25}R_{26}$, ureido, NH-CO-NHR_{24}, NR_{25}-CO-NHR_{24}, phosphato, $PR_{25}R_{24}$, $POR_{25}OR_{24}$, $P(=O)OR_{25}OR_{24}$, $OPR_{25}R_{24}$, $OPR_{25}OR_{24}$, $OP(=O)R_{25}OR_{24}$, OPO_3R_{25}, $OP(=O)OR_{25}OR_{24}$, SO_2R_{25}, sulfato, sulfo, R_{27}, N=N-R_{27}, or C_1-C_{12}alkoxy or C_1-C_{12}cycloalkoxy each unsubstituted or mono- or poly-substituted by halogen;

R_{19}, R_{20} and R_{23} are each independently of the others R_{16}, or C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_2-C_{12}alkenyl or C_3-C_{12}cycloalkenyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy radicals; or

R_{14} and R_{19} together, R_{15} and R_{19} together and/or R_{19} and R_{23} together are C_2-C_{12}alkylene, C_3-C_{12}cycloalkylene, C_2-C_{12}alkenylene or C_3-C_{12}cycloalkenylene, each of which is unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy radicals; or

R_{19} and R_{20} together with the common nitrogen are pyrrolidine, piperidine, piperazine or morpholine, each of which is unsubstituted or mono- to tetra-substituted by C_1-C_4alkyl; or carbazole, phenoxazine or phenothiazine, each of which is unsubstituted or substituted by one or more, where applicable identical or different,

radicals R_{28};

R_{21} and R_{22} are each independently of the other $NR_{25}R_{26}$, CN, $CONH_2$, $CONHR_{19}$, $CONR_{19}R_{20}$ or $COOR_{20}$;

R_{24}, R_{25} and R_{26} are each independently of the others C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_2-C_{12}alkenyl, C_3-C_{12}cycloalkenyl, C_6-C_{12}aryl, C_4-C_{12}heteroaryl, C_7-C_{12}aralkyl or C_5-C_{12}heteroaralkyl; or

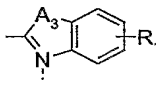
R_{25} and R_{26} together with the common nitrogen are pyrrolidine, piperidine, piperazine or morpholine, each of which is unsubstituted or mono- to tetra-substituted by C_1-C_4alkyl;

R_{27} is C_6-C_{12}aryl, C_4-C_{12}heteroaryl, C_7-C_{12}aralkyl or C_5-C_{12}heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18};

R_{28} is nitro, SO_2NHR_{25}, $SO_2NR_{25}R_{26}$, or C_1-C_{12}alkyl, C_3-C_{12}cycloalkyl, C_1-C_{12}alkylthio, C_3-C_{12}cycloalkylthio, C_1-C_{12}alkoxy or C_3-C_{12}cycloalkoxy, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17}; and

m is a number from 1 to 10.

2. An optical recording medium according to claim 1, wherein Q_1 and Q_2 are $C(R_{15})$;

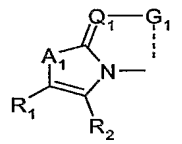
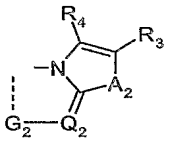
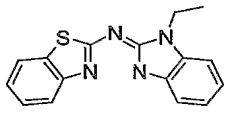
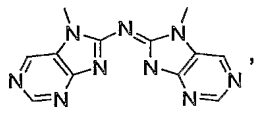
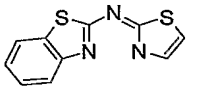
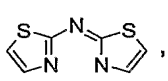
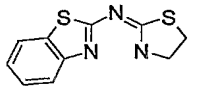
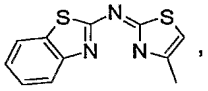
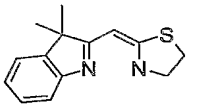
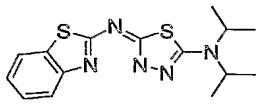
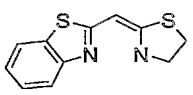
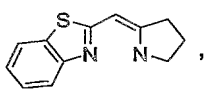
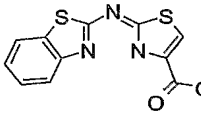
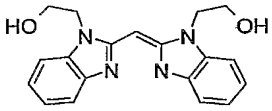
G_1 and G_2 are  ; and A_1, A_2 and A_3 are O, S or $N(R_{12})$;

R_{12} is C_1-C_{24}alkyl, C_1-C_4alkyl-[O-C_1-C_4alkylene]$_m$ or C_1-C_4alkyl-[NH-C_1-C_4alkylene]$_m$, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{17}, or C_6-C_{12}aryl unsubstituted or substituted by one or more, where applicable identical or different, radicals R_{18};

R_{15} is hydrogen, cyano, COO-R_{25} or C_1-C_{12}alkyl;

R_{17} is halogen, hydroxy, O-R_{25}, cyano, COO-R_{25} or carboxy; and

R_{18} is halogen, nitro, cyano, O-R_{19}, CH=C(CN)$_2$, COOR_{19}, ureido, CONH$R_{25}R_{26}$, SO_2R_{25}, P(=O)OR_{19}OR_{23} or unsubstituted or substituted C_1-C_{12}alkyl.

3. An optical recording medium according to claim 1 or 2, wherein the recording layer comprises a compound of formula (I) wherein  and/or  is/are  ,  ,  ,  ,  ,  ,  ,  ,  ,  ,  or  .

4. An optical recording medium according to claim 1, 2 or 3, wherein the compound of formula (I) contains branched C_3-C_{24}alkyl or branched C_3-C_{24}alkenyl.

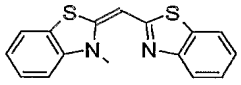
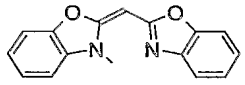
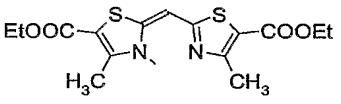
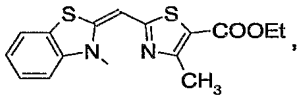
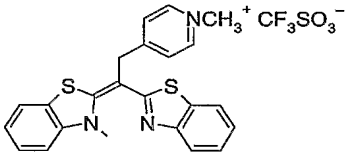
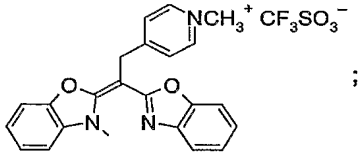
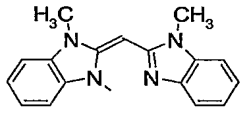
5. An optical recording medium according to claim 1, 2, 3 or 4, wherein the recording layer is substantially amorphous.

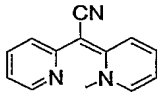
6. An optical recording medium according to claim 1, 2, 3, 4 or 5, additionally comprising a covering layer, wherein substrate, reflector layer, recording layer and covering layer are arranged in that order.

7. An optical recording medium according to claim 1, 2, 3, 4, 5 or 6, which in addition to comprising a compound of formula (I) comprises a metal-free chromophore.

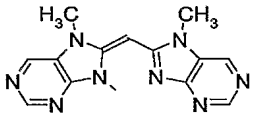
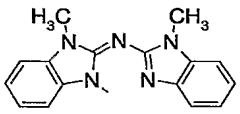
8. A method of recording or playing back data, wherein the data on an optical recording medium according to claim 1, 2, 3, 4, 5, 6 or 7 are recorded or played back at a wavelength of from 350 to 500 nm.

9. A compound of formula (I) according to claim 1, with the proviso that the compound is not a compound of formula $M_2(Z_1)_2$, wherein:

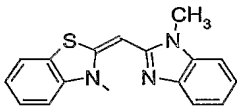
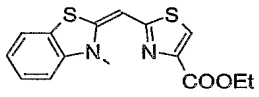
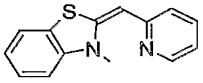
- M_2 is Co(II), Cu(II), Hg(II), Ni(II), Pd(II) or Zn(II) and Z_1 is  ;
- M_2 is Co(II), Cu(II), Ni(II), Pd(II) or Zn(II) and Z_1 is  ,  ,  ,  or  ;
- M_2 is Co(II), Cu(II), Ni(II) or Zn(II) and Z_1 is  ;

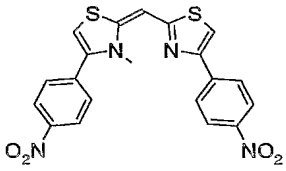
- M_2 is Cu(II), Pd(II) or Zn(II) and Z_1 is  ;

- M_2 is Co(II), Cu(II) or Zn(II) and Z_1 is

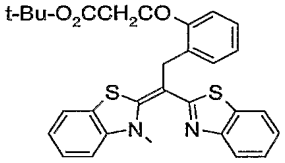
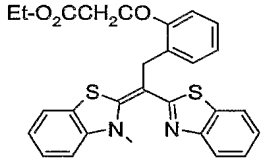
 or  ;

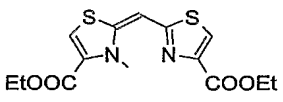
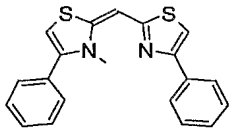
- M_2 is Cu(II) or Zn(II) and Z_1 is

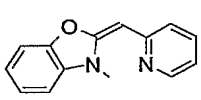
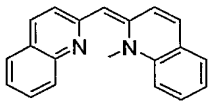
 ,  or  ;

- M_2 is Co(II) or Cu(II) and Z_1 is  ;

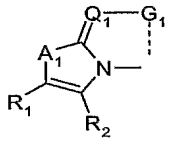
- M_2 is Pd(II) or Zn(II) and Z_1 is

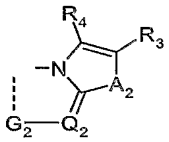
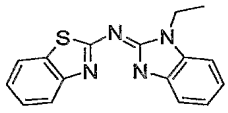
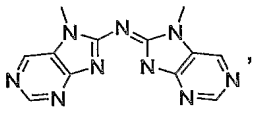
 or  ;

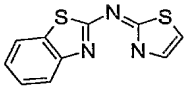
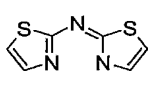
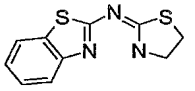
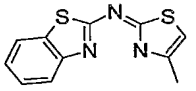
- M_2 is Cu(II) and Z_1 is  or  ; or

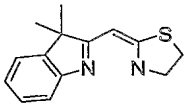
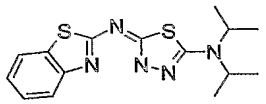
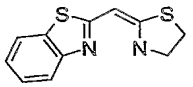
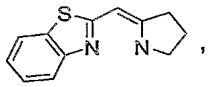
- M_2 is Zn(II) and Z_1 is  or  .

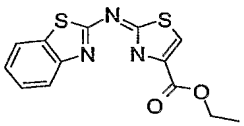
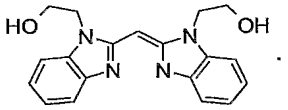
10. A compound according to claim 9, containing branched C_3-C_{24}alkyl or branched C_3-C_{24}alkenyl.

11. A compound according to claim 9 or 10 of formula (I), wherein 

and/or  is/are  ,  ,

 ,  ,  ,  ,

 ,  ,  ,  ,

 or  .

INTERNATIONAL SEARCH REPORT

International Application No
PCT/EP2004/050185

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 G11B7/24 C07D403/02

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 G11B C07D

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
EPO-Internal, WPI Data, PAJ, CHEM ABS Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	EP 1 130 584 A (MITSUI CHEMICAL) 5 September 2001 (2001-09-05) claim 1	1,8,9
A	US 5 962 657 A (H WOLLEB) 5 October 1999 (1999-10-05) column 3, line 28 - column 6, line 41; claim 1	1,8,9
A	DE 19 32 894 A (BASF) 28 January 1971 (1971-01-28) claim 1	9
A	US 6 376 664 B1 (M K CHAN) 23 April 2002 (2002-04-23) claims 1,2	9

☐ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

° Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

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"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
12 July 2004	21/07/2004

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Vanhecke, H

INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No
PCT/EP2004/050185

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DERWENT-ACC-NO: 2004-728406

DERWENT-WEEK: 200735

TITLE: Optical recording medium, e.g. compact disc for computer, includes recording layer comprising (new) transition metal complex of nitrogen-containing heterocyclic ligand

INVENTOR: BUDRY, J; LEHMANN, U ; SCHMIDHALTER, B ; SUTTER, P ; BUDRY, J L

PATENT-ASSIGNEE: CIBA SC HOLDING AG[CIBA] , CIBA SPECIALITY CHEM HOLDING INC[CIBA] , CIBA SPECIALTY CHEM HOLDING INC[CIBA] , BUDRY J[BUDRI] , LEHMANN U [LEHMI] , SCHMIDHALTER B[SCHMI] , SUTTER P [SUTTI]

PRIORITY-DATA: 2003CH-0000331 (March 3, 2003)

PATENT-FAMILY:

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DESIGNATED-STATES: AE AG AL AM AT AU AZ BA BB BG BR BW BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE EG ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NA NI NO NZ OM PG PH PL P T RO RU SC SD SE SG SK SL SY TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA ZM ZW AT BE BG BW CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS LU MC MW MZ NL OA PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE I T LI LT LU LV MC MK NL PT RO SE SI SK TR AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LU MC NL PT RO SE SI SK TR

APPLICATION-DATA:

PUB-NO	APPL-DESCRIPTOR	APPL-NO	APPL-DATE
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IN 200502505P4	N/A	2005IN-CN02505	October 3, 2005
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INT-CL (IPC): B32B003/02, B41M005/26 , C07D403/00 , C07D403/02 , C07F001/08 , C07F015/04 , C07F015/06 , C09B023/00 , C09B055/00 , C09B057/00 , C09B057/10 , G11B007/24 , G11B007/244

RELATED-ACC-NO: 2005-664282

ABSTRACTED-PUB-NO: WO2004079732A

BASIC-ABSTRACT:

NOVELTY - An optical recording medium comprises a substrate, a recording layer and optionally reflecting layer(s). The

recording layer comprises transition metal complex (I) of nitrogen-containing heterocyclic ligand, or its tautomer, some of which are new.

DETAILED DESCRIPTION - An optical recording medium comprises a substrate, a recording layer and optionally reflecting layer(s). The recording layer comprises a complex of formula (I) or its tautomer.

G1, G2 = a group of structures (IX)-(XII);

A1, A2 = N(R12), O, S or Se;

A3 = C(1-5C alkyl)2, C(4-5C alkylene), N(R12), O, S, Se, N=C (R13) or unsubstituted or R14-substituted CH=CH;

M1 = transition metal of groups IX-XII, preferably Co, Cu, Ni, Pd or Zn;

Q1, Q2 = C(R15), N or P;

R1-R8, R14 = H, R18, 6-12C aryl, 4-12C heteroaryl, 7-12C aralkyl or 5-12C heteroaralkyl, each optionally substituted by radicals R18;

R9, R12, R13 = 1-24C alkyl, 3-24C cycloalkyl, 2-24C alkenyl, 3-24C cycloalkenyl, 1-4C alkyl-(O-1-4C alkylene)O-1-4C alkylene)m or 1-4C alkyl-(NH-1-4C alkylene)m, each of which substituted by radicals R17; or 6-12C aryl, 4-12C heteroaryl, 7-12C aralkyl or 5-12C heteroaralkyl, each optionally substituted by radicals R18;

R10, R11, R18 = halo, nitro, cyano, thiocyano, hydroxy, O-R19, O-CO-R19, S-R19, CHO, COR20, CHOR19OR23, CR20OR19OR23, R16, N=N-R16, N=CR19R20, N=CR21R22, C(R15)=NR19, C(R15)=NR21, C(R15) =CR21R22, NH2, NH-R19, NR19R20, N=CR21R22, C(R15)=NR19, C(R15) =NR21, C(R15)=NR21R22, NH2, NH-R19, NR19R21, NH3+, NH2R19+, NHR19R20+, NR19R20R23+, CONH2, CONHR19, CONR19R20, SO2R19, SO2NH2, SO2NHR19, SO2NR19R20, COOH, COOR19, OCOOR19, NHCOR19, NR19COR23, NHCOOR19, NR19COOR23, ureido, NR19-CO-NHR23, B(OH)2, B (OH)(OR19), B(OR19)OR23, phosphato, PR19R23, POR19OR23, P(=O) OR19OR23, OPR19R23, OPR19OR23, OP(=O)R19OR23, OP(=O)OR19OR23, OPO3R19, sulfato, sulfo or 1-12C alkyl, 3-12C cycloalkyl, 1-12C alkylthio, 3-12C cycloalkylthio, 3-12C alkoxy or 3-12C cycloalkoxy, each optionally substituted by radicals R17;

R15 = H, cyano, hydroxy, 1-12C alkoxy, 3-12C cycloalkoxy, 1-12C alkylthio, 3-12C cycloalkylthio, amino, NHR24, NR25R26, R27, halo, nitro, formyl, N=N-R27, C(R14)=CR21R22, C(R14)=NR19, COO-R25, carboxy, carbamoyl, CONH-R25, CONR25R26, N=CR19R20, or 1-12C alkyl, 3-12C cycloalkyl, 2-12C alkenyl or 3-12C cycloalkenyl each optionally substituted by halo, hydroxy, 1-12C alkoxy or 3-12C cycloalkoxy;

R16 = 6-12C aryl, 4-12C heteroaryl, 7-12C aralkyl or 5-12C heteroaralkyl, each optionally substituted by radical R29;

R17 = halo, hydroxy, O-R25, O-CO-R25, S-R25, NH2, NH-R25, NR25R26, NH3+, NH2R25+, NHR25R26+, NR24R25R26+, NR25-CO-R24, NR25COOR24, cyano, formyl, COO-R25, carboxy, carbamoyl, CONH-R25, CONR25R26, ureido, NH-CO-NHR24, NR25-CO-NHR24, phosphato, PR25R24, POR25OR24, P(=O)OR25OR24, OPR25R24, OPR25OR24, OP(=O)R25OR24, OP(=O)OR25OR24, SO2R25, sulfato, sulfo, R27, N=N-R27 or 1-12C alkoxy or 1-12C cycloalkoxy each unsubstituted or mono- or poly-substituted by halo;

R19, R20, R23 = R16, or 1-12C alkyl, 3-12C cycloalkyl, 2-12C alkenyl, or 3-12C cycloalkenyl, each optionally substituted by halo, hydroxy, 1-12C alkoxy or 3-12C cycloalkoxy;

R21, R22 = NR25R26, CN, CONH2, CONHR19, CONR19R20 or COOR20;

R24-R26 = 1-12 alkyl, 3-12C cycloalkyl, 2-12C alkenyl, 3-12C cycloalkenyl, 6-12C aryl, 4-12C heteroaryl, 7-12C aralkyl or 5-12C heteroaralkyl;

R27 = 6-12C alkyl, 4-12C heteroalkyl, 7-12C aralkyl, or 5-12C heteroaralkyl, each optionally substituted by radicals R18;

R28 = nitro, SO2NHR25, SO2NR25R26, 1-12C alkyl, 3-12C cycloalkyl, 1-12C alkylthio, 3-12C cycloalkylthio, 1-12C alkoxy or 3-12C cycloalkoxy, each optionally substituted by radicals R17;

m = 1-10.

Optionally, R1+R2, R3+R4, R5+R6, R5+R13 and/or R5+R14 together in pairs are 3-6C alkylene or 3-6C alkenylene, each of which is optionally substituted by radicals R17 and may be interrupted by O, S or N(R12), or 1,4-buta-1,3-dienylene, groups of structure (1) or (2), each optionally substituted by radical R18 and in which 1 or 2 carbon atoms may have been replaced by nitrogen. R14

+R19, R15+R19 and/or R19+R23 together are 3-12C cycloalkyl, 2-12C alkenyl or 3-12C cycloalkenyl, each optionally substituted by halo, hydroxy, 1-12C alkoxy or 3-12C cycloalkoxy. R19+R20 together with the common nitrogen are pyrrolidine, piperidine, piperazine, or morpholine, each unsubstituted or mono- to tetra-substituted by 1-4C alkyl; or cabazole, phenoxazine or phenothiazine, each optionally substituted by radicals R28. R25 +R26 together with the common nitrogen are pyrrolidine, piperidine, piperazine or morpholine, each unsubstituted, or mono- to tetra-substituted by 1-4C alkyl.

INDEPENDENT CLAIMS are also included for:

(1) a method of recording or playing back data comprising recording or playing back the data on the optical recording medium at a wavelength of 350-500 nm; and

(2) new compounds (I) with the exception of those disclosed in J. Org. Chem. 67/16 5753-5772 (2002).

The new (I) are not e.g. compounds of formula M2(Z1)2 where M2 is Co(II), Cu(II), Hg(II), Ni(II), Pd(II) or Zn(II) and Z1 is a group of formula (a).

or where M2 is Co(II), Cu(II), Ni(II), Pd(II) or Zn(II) and Z1 is a group of formula (b)-(f).

Many other combinations of excluded metals and ligands are specified.

USE - The recording medium, e.g. compact disc or digital video disc, is used in computers and as storage material for identification and security cards or for the production of optical elements, e.g. holograms.

ADVANTAGE - The optical recording materials have excellent recording and playback quality especially at a wavelength of 350-500 nm. Recording and playback can be effected very advantageously with high sensitivity at the same wavelength, and the storage density is higher than in the case of known materials. The materials have very good storage properties before and after recording, even under especially harsh conditions, e.g. exposure to sunlight or fluorescent lighting, heat and/or high humidity. The manufacture is simple and readily reproducible using customary coating processes, e.g. spin-coating. The optical recording medium has high information

density, sensitivity and data reliability. It is robust, durable and easy to use. It is inexpensive to manufacture.

CHOSEN-DRAWING: Dwg.0/0

TITLE-TERMS: OPTICAL RECORD MEDIUM COMPACT DISC COMPUTER RECORD LAYER COMPRISE NEW TRANSITION METAL COMPLEX NITROGEN CONTAIN HETEROCYCLE LIGAND

DERWENT-CLASS: E12 L03 P73 P75 T03

CPI-CODES: E05-L; E05-M; E05-N; L03-G04B;

EPI-CODES: T03-B01B1; T03-B01D1; T03-B01D3;

CHEMICAL-CODES: Chemical Indexing M3 *01* Fragmentation Code A429 A960 C710 D012 D019 D022 D029 E600 E699 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M282 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHU8K AFHU8U

Chemical Indexing M3 *02* Fragmentation Code A429 A960 C710 D012 D019 E600 E699 K0 L3 L355 L9 L922 L999 M1 M126 M143 M280 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHUAK AFHUAU

Chemical Indexing M3 *03* Fragmentation Code A429 A960 C710 D012 D019 D022 D029 E400 E499 H7 H720 M1 M126 M132 M210 M214 M233 M240 M282 M311 M321 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHUCK AFHUCU

Chemical Indexing M3 *04* Fragmentation Code A428 A960 C710 D012 D019 D022 D029 E600 E699 H5 H542 H8 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M272 M282 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHULK AFHULU

Chemical Indexing M3 *05* Fragmentation Code A429 A960 C710 D012 D019 D022 D029 E600 E699 H5 H542 H8 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M272 M282 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHUNK AFHUNU

Chemical Indexing M3 *06* Fragmentation Code A429 A960 C316 C710 D012 D019 D022 D029 E600 E699 H7 H720 K0 K4 K442 K499 M1 M126 M132 M210 M212 M271 M282 M311 M321 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHURK AFHURU

Chemical Indexing M3 *07* Fragmentation Code A427 A960 C710 D012 D019 D022 D029 E600 E699 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M282 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHUTK AFHUTU

Chemical Indexing M3 *08* Fragmentation Code A427 A960 C710 D012 D019 D022 D029 E600 E699 H5 H542 H8 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M272 M282 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHUXK AFHUXU

Chemical Indexing M3 *09* Fragmentation Code A428 A960 C710 D012 D019 D022 D029 E600 E699 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M282 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHV0K AFHV0U

Chemical Indexing M3 *10* Fragmentation Code A428 A960 C316 C710 D012 D019 D022 D029 E400 E499 H7 H720 K0 K4 K442 K499 M1 M126 M132 M210 M212 M271 M282 M311 M321 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHV1K AFHV1U

Chemical Indexing M3 *11* Fragmentation Code A427 A960 C710 F012 F014 F019 F710 F799 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M282 M320 M411 M510 M522 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHV9K AFHV9U

Chemical Indexing M3 *12* Fragmentation Code A428 A960 C710 D012 D019 D022 D029 E600 E699 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M214

M233 M240 M282 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHVBK AFHVBU

Chemical Indexing M3 *13* Fragmentation Code A429 A960 C710 D012 D019 D022 D029 E600 E699 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M214 M233 M240 M282 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHVDK AFHVDU

Chemical Indexing M3 *14* Fragmentation Code A427 A960 C710 D012 D019 D022 D029 E600 E699 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M214 M233 M240 M282 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHVLK AFHVLU

Chemical Indexing M3 *15* Fragmentation Code A428 A960 C710 F012 F014 F019 F710 F799 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M282 M320 M411 M510 M522 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHVNK AFHVNU

Chemical Indexing M3 *16* Fragmentation Code A427 A960 C710 D012 D019 D022 D029 E400 E499 H7 H720 M1 M126 M132 M210 M214 M233 M240 M282 M311 M321 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHVPK AFHVPU

Chemical Indexing M3 *17* Fragmentation Code A429 A960 C710 F012 F014 F019 F710 F799 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M281 M320 M411 M510 M522 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHVWK AFHVWU

Chemical Indexing M3 *18* Fragmentation Code A428 A960 C710 F012 F014 F019 F710 F799 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M281 M320 M411 M510 M522 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHW1K AFHW1U

Chemical Indexing M3 *19* Fragmentation Code A427 A960 C710 F012 F014 F019 F710 F799 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M281 M320 M411 M510 M522 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHW6K AFHW6U

Chemical Indexing M3 *20* Fragmentation Code A428 A960 C710 D012 D019 E400 E499 H7 H720 M1 M126 M132 M280 M311 M321 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHW8K AFHW8U

Chemical Indexing M3 *21* Fragmentation Code A428 A960 C710 D012 D019 D022 D029 E400 E499 H7 H720 M1 M126 M132 M210 M214 M233 M240 M282 M311 M321 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHW9K AFHW9U

Chemical Indexing M3 *22* Fragmentation Code A427 A960 C710 D012 D019 E400 E499 H7 H720 M1 M126 M132 M280 M311 M321 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWCK AFHWCU

Chemical Indexing M3 *23* Fragmentation Code A427 A960 C710 D012 D019 E600 E699 K0 L3 L355 L9 L922 L999 M1 M126 M143 M280 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWDK AFHWDU

Chemical Indexing M3 *24* Fragmentation Code A428 A960 C710 D012 D019 E600 E699 K0 L3 L355 L9 L922 L999 M1 M126 M143 M280 M320 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWFK AFHWFU

Chemical Indexing M3 *25* Fragmentation Code A429 A960 C710 D012 D019 E400 E499 H7 H720 M1 M126 M132 M280 M311 M321 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWGK AFHWGU

Chemical Indexing M3 *26* Fragmentation Code A428 A960 C710 D012 D019 E400 E499 H7 H720 M1

M126 M132 M280 M312 M321 M331 M340 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWHK AFHWHU

Chemical Indexing M3 *27* Fragmentation Code A427 A960 C710 D012 D019 E400 E499 H7 H720 M1 M126 M132 M280 M312 M321 M331 M340 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWIK AFHWIU

Chemical Indexing M3 *28* Fragmentation Code A429 A960 C710 D012 D019 E400 E499 H7 H720 M1 M126 M132 M280 M312 M321 M331 M340 M343 M411 M512 M520 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWLK AFHWLU

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Chemical Indexing M3 *30* Fragmentation Code A428 A960 C710 F012 F015 F019 F710 F799 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M282 M320 M411 M510 M522 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWNK AFHWNU

Chemical Indexing M3 *31* Fragmentation Code A427 A960 C710 F012 F015 F019 F710 F799 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M282 M320 M411 M510 M522 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWOK AFHWOU

Chemical Indexing M3 *32* Fragmentation Code A429 A960 C710 F012 F015 F019 F710 F799 K0 L3 L355 L9 L922 L999 M1 M126 M143 M210 M211 M240 M282 M320 M411 M510 M522 M530 M540 M630 M781 M904 M905 Q454 R043 Specfic Compounds AFHWPK AFHWPU

Chemical Indexing M3 *33* Fragmentation Code A427 A428 A429 A430 A546 A960 B605 B615 B634

B701 B702 B712 B713 B720 B740 B741 B742 B743
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D013 D021 D022 D023 D700 F011 F012 F013 F014
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F423 F431 F432 F511 F512 F521 F522 F523 F530
F541 F542 F570 F580 F599 F610 F630 F699 F710
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G020 G021 G022 G029 G030 G031 G032 G039 G040
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G553 G563 H100 H101 H103 H121 H122 H123 H161
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H621 H622 H623 H721 J011 J012 J013 J014 J111
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J412 J581 J582 J583 K421 K431 K499 K534 K599
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L660 L699 L722 L724 L910 L921 L922 L941 L943
L999 M1 M113 M115 M116 M119 M123 M125 M126 M129
M132 M135 M139 M141 M142 M143 M144 M149 M150
M210 M211 M212 M213 M214 M215 M216 M220 M221
M222 M223 M224 M225 M226 M231 M232 M233 M240
M262 M263 M271 M272 M273 M280 M281 M282 M283
M311 M312 M313 M314 M315 M316 M320 M321 M322
M323 M331 M332 M333 M340 M342 M343 M373 M391
M392 M393 M411 M510 M511 M521 M522 M523 M530
M531 M532 M533 M540 M541 M542 M543 M630 M781
M904 M905 Q454 R043 Ring Index 00085 00090
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Markush Compounds 200140-51401-K 200140-51401-U

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